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## Contributions to discriminant analysis

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CONTRIBUTIONS TO DISCRIMINANT ANALYSIS

by

Nell Sedransk

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## INTRODUCTION

The discrimination problem, most simply explained, consists of deciding how to assign a single observed element,  $X$ , to one of two or more different populations. It is assumed, a priori, that  $X$  comes from one of these populations. The more particular discrimination problem treated here considers only two populations. These populations,  $\pi_1$  and  $\pi_2$ , are assumed to be  $p$ -dimensional normal with mean vectors,  $\mu_1$  and  $\mu_2$ , and common covariance matrix  $\Sigma$ . The parameters  $\mu_1$  and  $\mu_2$  are assumed to be unknown; the cases  $\Sigma$  known and  $\Sigma$  unknown are considered. To estimate the unknown parameters, previously obtained observations  $x_{1i}$  ( $i = 1, 2, \dots, n_1$ ) from  $\pi_1$  and  $x_{2j}$  ( $j = 1, 2, \dots, n_2$ ) from  $\pi_2$  are used. The discrimination problem is further limited by requiring that a linear function of  $X$  be used to determine the assignment of  $X$  to either  $\pi_1$  or  $\pi_2$ . The ideal case, when no parameters need be estimated, has a single admissible solution; that is (assuming no a priori probabilities of origin are available) a solution which minimizes the probability of assigning  $X$  to  $\pi_2$  when it comes from  $\pi_1$  and the probability of assigning  $X$  to  $\pi_1$  when it comes from  $\pi_2$ . This solution is to assign  $X$  to  $\pi_1$  or  $\pi_2$  as the function  $V = [X - \frac{1}{2}(\mu_1 + \mu_2)]' \Sigma^{-1} [\mu_1 - \mu_2]$  is positive or negative.

The usual discrimination function for the case when  $\mu_1$  and  $\mu_2$  are unknown and  $\Sigma$  is known is obtained by modifying the function  $V$  by

substituting the sample means,  $\bar{x}_1$  and  $\bar{x}_2$ , for the parameters  $\mu_1$  and  $\mu_2$ . As the function  $[X - \frac{1}{2}(\bar{x}_1 + \bar{x}_2)]' \Sigma^{-1} [\bar{x}_1 - \bar{x}_2]$ , where

$$\bar{x}_1 = n_1^{-1} \sum_{i=1}^{n_1} x_{1i} \text{ and } \bar{x}_2 = n_2^{-1} \sum_{j=1}^{n_2} x_{2j}, \text{ is positive or negative, } X$$

is assigned to  $\pi_1$  or  $\pi_2$ . When no parameter values are known, the

function  $V$  is further modified by estimating  $\Sigma$  in the usual manner,

giving  $[X - \frac{1}{2}(\bar{x}_1 + \bar{x}_2)]' S^{-1} [\bar{x}_1 - \bar{x}_2]$ , where

$$S = (n_1 + n_2 - 2)^{-1} \left[ \sum_{i=1}^{n_1} (x_{1i} - \bar{x}_1)(x_{1i} - \bar{x}_1)' + \sum_{j=1}^{n_2} (x_{2j} - \bar{x}_2)(x_{2j} - \bar{x}_2)' \right],$$

which is variously identified in the literature as the "Fisherian discrim-

inant function" (for Fisher who suggested it (1936)), "Anderson's  $W$ ,"

or more simply " $W$ " (for Wald who first investigated its properties (1944)).

In the processes described above the "discrimination point" is zero

(i.e., as the appropriate function is greater than or less than zero,  $X$

is assigned to  $\pi_1$  or  $\pi_2$ ). When all parameters have known values,

zero is the optimal choice as the discrimination point. When some or all

of the parameters are estimated, the use of zero as the discrimination

point is largely an intuitive choice or a matter of convenience. The topic

dealt with in Part I of this dissertation is the choice of the discrimination

point. It seems logical that if  $\mu_1$  and  $\mu_2$  are estimated with differing

degrees of precision, the discrimination point should not be placed sym-

metrically; rather, its position should reflect the relative precisions of

the estimators. The results obtained in Part I indicate that a discrimina-

tion point of  $-\frac{1}{2}(n_1^{-1} - n_2^{-1})(p-2)$ , where  $p$  denotes the dimensionality

of  $\pi_1$  and  $\pi_2$ , reduces the combined probabilities of misclassification from those associated with a discrimination point of zero.

Once a discrimination or classification procedure has been determined, the probability of a particular kind of error (e.g., assigning  $X$  to  $\pi_1$  when, in fact,  $X$  comes from  $\pi_2$ ) may be of interest. More precisely, the probability of a particular kind of error, conditional upon the sample values ( $\bar{x}_1$ ,  $\bar{x}_2$  and  $S$  also if  $\Sigma$  is unknown) used to define the procedure, may be of interest. This probability is a function of the sizes,  $n_1$  and  $n_2$ , of the samples used to estimate the unknown parameters of  $\pi_1$  and  $\pi_2$ , and of the Mahalanobis distance between  $\pi_1$  and  $\pi_2$ , given by  $D^2 = (\mu_1 - \mu_2)' \Sigma^{-1} (\mu_1 - \mu_2)$ , a function of the unknown parameters. Part II deals with the problem of estimating this (conditional) probability of a particular kind of error. At least fifteen different estimators appear in the literature. Some of these are equally adaptable to non-normal populations; but more of them rely upon the assumption of the normality of  $\pi_1$  and  $\pi_2$ . The reasoning underlying them is variously intuitive, classical, and Bayesian. The most promising of each type as well as the most commonly used are investigated here. Unconditional mean square error is the criterion for comparison. Mean square error was chosen as a relatively "fair" way to assess the behavior of both Bayesian and non-Bayesian estimators. Unconditional mean square error was chosen because someone applying a fixed

classification procedure is undoubtedly interested in estimating the conditional probability of misclassification, but his choice of an estimator might well be based on a variety of possible true (if unknown) conditions. (Because of the intractability of the precise distribution of  $W$ , the results obtained are based on an asymptotic expansion for the distribution.) The relative performances of the groups of estimators might be anticipated. Estimators requiring fewer initial assumptions (notably, the normality of  $\pi_1$  and  $\pi_2$ ) have larger mean square errors than do those relying on knowledge of the distributions involved. Also, differences in mean square errors within types of estimators decrease as the sample sizes increase.

The topic treated in Part III is the characterization of populations  $\pi_1$  and  $\pi_2$  to simultaneously reduce the number of dimensions to be considered and to differentiate as sharply as possible between  $\pi_1$  and  $\pi_2$ . It is no longer assumed that the populations are normally distributed; and complex-valued variables are considered. A defense of the extension of usual methods to the complex case is presented.



PART I. CHOICE OF A DISCRIMINATION POINT

## CLASSICAL APPROACH TO THE PROBLEM

### Linear Discriminant Function

The general two population discrimination problem consists of deciding how to assign a single observed element  $X$  to one of two populations,  $\pi_1$  and  $\pi_2$ . It is assumed that the assignment of  $X$  must be based on a linear function of its (single- or vector-) value and any knowledge about the parameters of  $\pi_1$  and  $\pi_2$ , but not on any subjective (or other) prior probabilities. It is further assumed that the assignment of  $X$  cannot be deferred.

Let  $x_{1i}$  ( $i = 1, 2, \dots, n_1$ ) and  $x_{2j}$  ( $j = 1, 2, \dots, n_2$ ) denote two independent random samples from  $p$ -dimensional normal populations with means  $\mu_1$  and  $\mu_2$  and common covariance matrix  $\Sigma$ . Let  $X$  be a subsequently and independently (of the  $x_{1i}$  and of the  $x_{2j}$ ) drawn observation from either  $\pi_1$  or  $\pi_2$ .

If all parameter values are known, then there is a "best" procedure. "Best" in this context means: (1) admissible, (2) unique Bayes' under equal a priori probabilities of  $\pi_1$  and  $\pi_2$  and under equal losses for the two kinds of errors possible, or (3) minimax. Wald (1944) derives this procedure by seeking the method of classification that is "best" in the sense of (2). Letting  $f_1(X)$  denote the density function of  $X$  when  $X$  comes from  $\pi_1$  and letting  $f_2(X)$  denote the density function of  $X$  when  $X$  comes from  $\pi_2$ , the conditional density, denoted by  $q_1(X)$ , of

originating in  $\pi_1$  given  $X$  can be written

$$(1.1) \quad q_1(X) = f_1(X)[f_1(X) + f_2(X)]^{-1}.$$

Similarly, the conditional density, denoted by  $q_2(X)$ , of originating in  $\pi_2$  given  $X$  can be written

$$(1.2) \quad q_2(X) = f_2(X)[f_1(X) + f_2(X)]^{-1}.$$

To minimize the probability of misclassification (both of classifying  $X$  as belonging to  $\pi_2$  when  $X$  comes from  $\pi_1$  and of classifying  $X$  as belonging to  $\pi_1$ , then  $X$  comes from  $\pi_2$ ),  $X$  is assigned to  $\pi_1$  or to  $\pi_2$  as  $q_1(X)$  or  $q_2(X)$ , respectively, is the larger. This manner of assigning  $X$  to  $\pi_1$  or to  $\pi_2$  is equivalent to examining

$$(1.3) \quad \frac{q_1(X)}{q_2(X)} = \frac{f_1(X)}{f_2(X)}$$

and assigning  $X$  to  $\pi_1$  or to  $\pi_2$  as this ratio is greater than or less than one. When both  $\pi_1$  and  $\pi_2$  are multivariate normal populations (as specified above, with differing means  $\mu_1$  and  $\mu_2$  and with common covariance matrix  $\Sigma$ ) the ratio of densities given in equation 1.3 reduces to

$$(1.4) \quad \frac{q_1(X)}{q_2(X)} = \exp \left\{ -\frac{1}{2}(X-\mu_1)' \Sigma^{-1}(X-\mu_1) + \frac{1}{2}(X-\mu_2)' \Sigma^{-1}(X-\mu_2) \right\}.$$

By taking the logarithm (a monotonic increasing function) of equation 1.4, it follows that this assignment procedure is equivalent to

$$(1.5) \quad \text{Classify } X \text{ as belonging to } \pi_1 \text{ when}$$

$$-\frac{1}{2}(X-\mu_1)' \Sigma^{-1}(X-\mu_1) + \frac{1}{2}(X-\mu_2)' \Sigma^{-1}(X-\mu_2) \geq 0;$$

otherwise classify  $X$  as belonging to  $\pi_2$ .

Rearrangement of the expression in procedure 1.5 gives the familiar expression, denoted by  $V$ , and the procedure

(1.6) Classify  $X$  as belonging to  $\pi_1$  or  $\pi_2$  as

$$V = X' \Sigma^{-1} (\mu_1 - \mu_2) - \frac{1}{2} (\mu_1 + \mu_2)' \Sigma^{-1} (\mu_1 - \mu_2)$$

is positive or negative.

Wald (1944), Anderson (1958) and Rao (1965) discuss this procedure. For proofs of other properties, see Anderson (1958).

When, as is more often the case, the parameter values are unknown a like procedure seems intuitively reasonable; but its properties are no longer so easily ascertained. A direct manner of obtaining the linear discriminant function  $W$  is to substitute the usual sample estimates for the unknown parameters into the expression for  $V$  in procedure 1.6. Thus the following classification procedure is derived.

(1.7) Classify  $X$  as belonging to  $\pi_1$  and  $\pi_2$  as

$$W = X' S^{-1} (\bar{x}_1 - \bar{x}_2) - \frac{1}{2} (\bar{x}_1 + \bar{x}_2)' S^{-1} (\bar{x}_1 - \bar{x}_2)$$

is positive or negative,

where  $\bar{x}_1 = n_1^{-1} \sum_{i=1}^{n_1} x_{1i}$ ,  $\bar{x}_2 = n_2^{-1} \sum_{j=1}^{n_2} x_{2j}$ , and

$$S = (n_1 + n_2 - 2)^{-1} \left[ \sum_{i=1}^{n_1} (x_{1i} - \bar{x}_1)(x_{1i} - \bar{x}_1)' + \sum_{j=1}^{n_2} (x_{2j} - \bar{x}_2)(x_{2j} - \bar{x}_2)' \right].$$

This procedure seems intuitively reasonable, and one might hope that it would give good results since it approximates the excellent procedure 1.6.

Fisher (1936) derived the first term of  $W$  and an analogous procedure to procedure 1.7 by using a regression technique and a dummy variable. Define  $y_{1i}$  ( $i = 1, 2, \dots, n_1$ ) and  $y_{2j}$  ( $j = 1, 2, \dots, n_2$ ) by

$$(1.8) \quad y_{1i} = n_2(n_1 + n_2)^{-1} \quad \text{for } i = 1, 2, \dots, n_1; \text{ and}$$

$$y_{2j} = -n_1(n_1 + n_2)^{-1} \quad \text{for } j = 1, 2, \dots, n_2.$$

(Thus a positive  $y$  value is associated with  $\pi_1$  and a negative  $y$  value is associated with  $\pi_2$ .) An artificial model can be applied to the  $y_{k\ell}$  ( $k = 1, 2; \ell = 1, 2, \dots, n_k$ ). Consider the model below.

$$(1.9) \quad y_{k\ell} = \beta' [x_{k\ell} - (n_1 + n_2)^{-1}(n_1 \bar{x}_1 + n_2 \bar{x}_2)] + \epsilon_{k\ell}$$

for  $k = 1, 2; \ell = 1, 2, \dots, n_k$ ,

where  $y_{k\ell}$  is a scalar (assuming the two values given in equation 1.8),  $\beta'$  is a  $1 \times p$  vector of regression coefficients, the  $x_{k\ell}$  are the  $p \times 1$  vector observations from  $\pi_1$  and  $\pi_2$ , and  $\bar{x}_1$  and  $\bar{x}_2$  are  $p \times 1$  vector sample means, defined below procedure 1.7, and the  $\epsilon_{k\ell}$  are the (scalar) residuals. The usual least squares technique gives the solution

$$(1.10) \quad \hat{\beta} \propto S^{-1}(\bar{x}_1 - \bar{x}_2).$$

Substituting this solution into the model gives

$$(1.11) \quad y_{k\ell} = (\bar{x}_1 - \bar{x}_2)' S^{-1} [x_{k\ell} - (n_1 + n_2)^{-1}(n_1 \bar{x}_1 + n_2 \bar{x}_2)] + \epsilon_{k\ell}$$

Using equation 1.11 as a predictive equation results in predicting  $y$  to be positive (associated with  $\pi_1$ ) or negative (associated with  $\pi_2$ ) as  $X'S^{-1}(\bar{x}_1 - \bar{x}_2)$  is greater than or less than a constant. Thus, letting  $y$  represent the assignment of  $X$

(to  $\pi_1$  when  $y$  is positive, to  $\pi_2$  when  $y$  is negative), a procedure analogous to procedure 1.7 is defined.

The distribution of the statistic  $W$  as defined in procedure 1.7 is quite complicated, and depends on  $n_1, n_2$  and Mahalanobis' distance, denoted by  $D^2$  and given by

$$(1.12) \quad D^2 = (\mu_1 - \mu_2)' \Sigma^{-1} (\mu_1 - \mu_2).$$

Wald (1944), Anderson (1951), Sitgreaves (1952), Kabe (1963), and Okamoto (1963) have all studied the distribution of  $W$ . The earliest analytic support for procedure 1.7 was given by Wald (1944). He used large sample theory to show that the limiting distribution of  $W$  is that of  $V$ .

#### Probabilities of Misclassification

Several types of probabilities of misclassification are of interest. The first, denoted by  $P^{**}$ , is the probability of misclassification in optimal circumstances (i.e., when all parameters of  $\pi_1$  and  $\pi_2$  have known values).

$$(1.13) \quad P_1^{**} = \Pr \{X \text{ classified as belonging to } \pi_2 \mid \mu_1, \mu_2, \Sigma \text{ known, } X \in \pi_1\}; \text{ and}$$

$$P_2^{**} = \Pr \{X \text{ classified as belonging to } \pi_1 \mid \mu_1, \mu_2, \Sigma \text{ known, } X \in \pi_2\}.$$

A second probability of misclassification, denoted by  $P^*$ , is the unconditional probability of misclassification when the parameter values are

unknown.

$$(1.14) \quad P_1^* = \Pr \{X \text{ classified as belonging to } \pi_2 \mid X \in \pi_1\}; \text{ and}$$

$$P_2^* = \Pr \{X \text{ classified as belonging to } \pi_1 \mid X \in \pi_2\}.$$

The remaining probability of misclassification, denoted by  $P$ , is the conditional (on  $\bar{x}_1$ ,  $\bar{x}_2$  and  $S$ ) probability of misclassification when the unknown parameter values are estimated by  $\bar{x}_1$ ,  $\bar{x}_2$  and  $S$ .

$$(1.15) \quad P_1 = \Pr \{X \text{ classified as belonging to } \pi_2 \mid \bar{x}_1, \bar{x}_2, S, X \in \pi_1\}; \text{ and}$$

$$P_2 = \Pr \{X \text{ classified as belonging to } \pi_1 \mid \bar{x}_1, \bar{x}_2, S, X \in \pi_2\}.$$

When all parameter values are known and procedure 1.6 is used, only the probabilities of misclassification  $P_1^{**}$  and  $P_2^{**}$  are relevant. These are relatively easy to determine. Note that the distribution of  $V$  is  $N(\frac{1}{2}D^2, D^2)$  or  $N(-\frac{1}{2}D^2, D^2)$  as  $X$  comes from  $\pi_1$  or  $\pi_2$ , where  $N(\nu, \psi^2)$  denotes the distribution of a (scalar) normal variable with mean  $\nu$  and variance  $\psi^2$ . It follows that

$$(1.16) \quad P_1^{**} = \Pr \{V \leq 0 \mid X \in \pi_1\}; \text{ and}$$

$$P_2^{**} = \Pr \{V > 0 \mid X \in \pi_2\},$$

and hence, that

$$(1.17) \quad P_1^{**} = \Phi(-\frac{1}{2}D); \text{ and}$$

$$P_2^{**} = \Phi(-\frac{1}{2}D),$$

where  $\Phi$  is the cumulative distribution function of a standard normal

variable.

When the parameter values are unknown, the conditional probabilities of misclassification,  $P_1$  and  $P_2$ , and the unconditional probabilities of misclassification,  $P_1^*$  and  $P_2^*$ , are of interest. The appropriate procedure for this case is procedure 1.7, which leads to the conditional probabilities of misclassification given by

$$(1.18) \quad P_1 = \Pr \{W \leq 0 \mid \bar{x}_1, \bar{x}_2, S, X \in \pi_1\}, \text{ and} \\ P_2 = \Pr \{W > 0 \mid \bar{x}_1, \bar{x}_2, S, X \in \pi_2\}.$$

Since the conditional distribution of  $W$  given  $\bar{x}_1, \bar{x}_2$  and  $S$  is

$$N\left(\left[\mu_1 - \frac{1}{2}(\bar{x}_1 + \bar{x}_2)'\right] S^{-1}(\bar{x}_1 - \bar{x}_2), (\bar{x}_1 - \bar{x}_2)' S^{-1} \Sigma S^{-1}(\bar{x}_1 - \bar{x}_2)\right) \\ \text{or } N\left(\left[\mu_2 - \frac{1}{2}(\bar{x}_1 + \bar{x}_2)'\right] S^{-1}(\bar{x}_1 - \bar{x}_2), (\bar{x}_1 - \bar{x}_2)' S^{-1} \Sigma S^{-1}(\bar{x}_1 - \bar{x}_2)\right)$$

as  $X$  comes from  $\pi_1$  or  $\pi_2$ , equations 1.18 can be written

$$(1.19) \quad P_1 = \Phi \left[ - \frac{(\mu_1 - \frac{1}{2}[\bar{x}_1 + \bar{x}_2])' \Sigma^{-1}(\bar{x}_1 - \bar{x}_2)}{[(\bar{x}_1 - \bar{x}_2)' S^{-1} \Sigma S^{-1}(\bar{x}_1 - \bar{x}_2)]^{1/2}} \right], \text{ and} \\ P_2 = \Phi \left[ \frac{(\mu_2 - \frac{1}{2}[\bar{x}_1 + \bar{x}_2])' \Sigma^{-1}(\bar{x}_1 - \bar{x}_2)}{[(\bar{x}_1 - \bar{x}_2)' S^{-1} \Sigma S^{-1}(\bar{x}_1 - \bar{x}_2)]^{1/2}} \right].$$

It is not possible to produce immediately a specific version of equations 1.19 in terms of the parameters of  $\pi_1$  and  $\pi_2$ . Nor, since the distribution of  $W$  is intractable, is it easy to obtain expressions for  $P_1^*$  and  $P_2^*$ . It can be noted, however, that  $P_1$  and  $P_2$  are unbiased estimators for  $P_1^*$  and  $P_2^*$ , respectively.



## SUGGESTED DISCRIMINATION POINT

## Derivation

Because of the intractability of the distribution of  $W$ , little evaluation of the classification procedure 1.7 (with regard to  $P_1^*$  and  $P_2^*$ ) is given in the literature. The choice of zero as a discrimination point (i.e., classifying  $X$  as belonging to  $\pi_1$  or  $\pi_2$  as  $W$  is greater than or less than zero) is not discussed. With the availability of Okamoto's (1963) asymptotic expansion for the distribution of  $W$ , an evaluation of discrimination points is possible. That zero might sometimes prove an inferior choice seems likely. For example, when the sample sizes,  $n_1$  and  $n_2$ , are fairly small and quite unequal,  $\mu_1$  and  $\mu_2$  are estimated with differing precision. In applying procedure 1.7, one is, in fact, using  $\bar{x}_1$  and  $\bar{x}_2$  (and  $S$ ) as if the parameter values of  $\pi_1$  and  $\pi_2$  are  $\bar{x}_1$ ,  $\bar{x}_2$  and  $S$ . When, for example,  $\mu_2$  is estimated quite precisely while  $\mu_1$  is estimated on the basis of very few observations, it seems illogical to put equal faith in the estimates and to adopt the symmetric (with respect to  $\bar{x}_1$  and  $\bar{x}_2$ ) procedure 1.7.

The method used here to obtain a desirable discrimination point,  $k_0$ , is to minimize over  $k$  the combined probability of misclassification.

Let the classification procedure be given by

- (1.20)      Classify  $X$  as belonging to  $\pi_1$  whenever  $W \geq k$ ;  
                  classify  $X$  as belonging to  $\pi_2$  whenever  $W < k$ ,

and let  $H(k)$  be defined by

$$(1.21) \quad H(k) = P_1^*(k) + P_2^*(k)$$

where  $P_i^*(k)$  denotes  $P_i^*$  under the classification procedure 1.20. Thus the problem here is to find  $k_0$  such that

$$(1.22) \quad H(k_0) = \min_k H(k).$$

Following procedure 1.20 leads to the combined (unconditional) probability of misclassification given by

$$(1.23) \quad H(k) = \Pr \{W < k \mid X \in \pi_1\} + \Pr \{W \geq k \mid X \in \pi_2\}.$$

Making use of Okamoto's (1963) asymptotic expansion, equation 1.23 can be rewritten explicitly up to terms of the second order of  $n_1^{-1}$ ,  $n_2^{-1}$  and  $(n_1 + n_2 - 2)^{-1}$  as

$$(1.24) \quad H(k) = \Phi\left(\frac{k}{D} - \frac{D}{2}\right) + \left( [2n_1 D^2]^{-1} \left[ 3\left(\frac{k}{D} - \frac{D}{2}\right) - \left(\frac{k}{D} - \frac{D}{2}\right)^3 - p\left(\frac{k}{D} - \frac{3D}{2}\right) \right] \right. \\ \left. + [2n_2 D^2]^{-1} \left[ 2D + 3\left(\frac{k}{D} - \frac{D}{2}\right) - \left(\frac{k}{D} - \frac{D}{2}\right)\left(\frac{k}{D} + \frac{D}{2}\right)^2 - p\left(\frac{k}{D} + \frac{D}{2}\right) \right] \right) \cdot \phi\left(\frac{k}{D} - \frac{D}{2}\right) \\ + \Phi\left(-\frac{k}{D} - \frac{D}{2}\right) + \left( [2n_1 D^2]^{-1} \left[ 2D - 3\left(\frac{k}{D} + \frac{D}{2}\right) + \left(\frac{k}{D} + \frac{D}{2}\right)\left(\frac{k}{D} - \frac{D}{2}\right)^2 + p\left(\frac{k}{D} - \frac{D}{2}\right) \right] \right. \\ \left. + [2n_2 D^2]^{-1} \left[ -3\left(\frac{k}{D} + \frac{D}{2}\right) + \left(\frac{k}{D} + \frac{D}{2}\right)^3 + p\left(\frac{3D}{2} + \frac{k}{D}\right) \right] \right) \phi\left(-\frac{k}{D} - \frac{D}{2}\right) + O_2$$

where  $\phi$  is the density function of a standard normal variable and where  $O_2$  denotes second order terms of  $n_1^{-1}$ ,  $n_2^{-1}$  and  $(n_1 + n_2 - 2)^{-1}$ .

For convenience in dealing with equation 1.24, define  $f(k)$  and  $g(k)$  by

$$(1.25) \quad f(k) = \Phi\left(\frac{k}{D} - \frac{D}{2}\right) + \Phi\left(-\frac{k}{D} - \frac{D}{2}\right); \text{ and}$$

$$(1.26) \quad g(k) = \left( [2n_1 D^2]^{-1} \left[ 3\left(\frac{k}{D} - \frac{D}{2}\right) - \left(\frac{k}{D} - \frac{D}{2}\right)^3 - p\left(\frac{k}{D} + \frac{D}{2}\right) \right] \right. \\ \left. + [2n_2 D^2]^{-1} \left[ 2D + 3\left(\frac{k}{D} - \frac{D}{2}\right) - \left(\frac{k}{D} - \frac{D}{2}\right)\left(\frac{k}{D} + \frac{D}{2}\right)^2 - p\left(\frac{k}{D} - \frac{D}{2}\right) \right] \right) \cdot \\ \cdot \Phi\left(\frac{k}{D} - \frac{D}{2}\right) \\ + \left( [2n_1 D^2]^{-1} \left[ 2D - 3\left(\frac{k}{D} + \frac{D}{2}\right) + \left(\frac{k}{D} + \frac{D}{2}\right)\left(\frac{k}{D} - \frac{D}{2}\right)^2 - p\left(\frac{k}{D} - \frac{D}{2}\right) \right] \right. \\ \left. + [2n_2 D^2]^{-1} \left[ -3\left(\frac{k}{D} + \frac{D}{2}\right) + \left(\frac{k}{D} + \frac{D}{2}\right)^3 + p\left(\frac{k}{D} + \frac{3D}{2}\right) \right] \right) \Phi\left(-\frac{k}{D} - \frac{D}{2}\right).$$

To find the derivative of  $H(k)$  (as given by equation 1.24) consider first the derivative of  $f(k)$  (as given by equation 1.25). It is quickly established that

$$(1.27) \quad f'(k) = D^{-1} \phi\left(\frac{k}{D} - \frac{D}{2}\right) - D^{-1} \phi\left(-\frac{k}{D} - \frac{D}{2}\right).$$

The derivative of  $g(k)$  (defined by equation 1.26) after some tedious algebra can be shown to be

$$(1.28) \quad g'(k) = \left( [2n_1 D^3]^{-1} \left[ 3-p-(6-p)\left(\frac{k}{D} - \frac{D}{2}\right)^2 + \left(\frac{k}{D} - \frac{D}{2}\right)^4 - p\left(k - \frac{D^2}{2}\right) \right] \right. \\ \left. + [2n_2 D^3]^{-1} \left[ 3-p-D^2-(6-p)\left(\frac{k}{D} + \frac{D}{2}\right)\left(\frac{k}{D} - \frac{D}{2}\right) + \left(\frac{k}{D} + \frac{D}{2}\right)^2 \left(\frac{k}{D} - \frac{D}{2}\right)^2 \right] \right) \phi\left(\frac{k}{D} - \frac{D}{2}\right) \\ + \left( [2n_1 D^3]^{-1} \left[ -(3-p)+D^2 + (6-p)\left(\frac{k}{D} + \frac{D}{2}\right)\left(\frac{k}{D} - \frac{D}{2}\right) - \left(\frac{k}{D} + \frac{D}{2}\right)^2 \left(\frac{k}{D} - \frac{D}{2}\right)^2 \right] \right. \\ \left. + [2n_2 D^3]^{-1} \left[ -(3-p) + (6-p)\left(\frac{k}{D} + \frac{D}{2}\right)^2 - \left(\frac{k}{D} + \frac{D}{2}\right)^4 - p\left(\frac{k}{D} + \frac{D}{2}\right) \right] \right) \phi\left(-\frac{k}{D} - \frac{D}{2}\right).$$

From equations 1.27 and 1.28 is obtained

$$\begin{aligned}
(1.29) \quad H'(k) = & \left( 1 + [2n_1 D^3]^{-1} [3-p-(6-p)\left(\frac{k}{D}-\frac{D}{2}\right)^2 + \left(\frac{k}{D}-\frac{D}{2}\right)^4 - p\left(k-\frac{D^2}{2}\right)] \right. \\
& + [2n_2 D^3]^{-1} [3-p-D^2-(6-p)\left(\frac{k}{D}+\frac{D}{2}\right)\left(\frac{k}{D}-\frac{D}{2}\right) + \left(\frac{k}{D}+\frac{D}{2}\right)^2 \left(\frac{k}{D}-\frac{D}{2}\right)^2] \left. \right) \phi\left(\frac{k}{D}-\frac{D}{2}\right) \\
& - \left( 1 + [2n_1 D^3]^{-1} [3-p-D^2-(6-p)\left(\frac{k}{D}+\frac{D}{2}\right)\left(\frac{k}{D}-\frac{D}{2}\right) + \left(\frac{k}{D}+\frac{D}{2}\right)^2 \left(\frac{k}{D}-\frac{D}{2}\right)^2] \right. \\
& + [2n_2 D^3]^{-1} [3-p-(6-p)\left(\frac{k}{D}+\frac{D}{2}\right)^2 + \left(\frac{k}{D}+\frac{D}{2}\right)^4 + p\left(k+\frac{D^2}{2}\right)] \left. \right) \phi\left(-\frac{k}{D}-\frac{D}{2}\right).
\end{aligned}$$

Setting equation 1.29 equal to zero and solving for  $k$  yields no immediate solution. Note that  $H'(k)$  is a complicated expression with each of  $\phi\left(\frac{k}{D}-\frac{D}{2}\right)$  and  $\phi\left(-\frac{k}{D}-\frac{D}{2}\right)$  multiplied by a fourth degree polynomial in  $k$ . Investigation shows that it is not certain that either of these polynomials has a real root, nor that a weighted difference of these two polynomials has a real root. The only property of a solution to the equation  $H'(k) = 0$  which is immediately apparent is its dependence on  $n_1$ ,  $n_2$ ,  $p$  and  $D^2$ . Moreover,  $D^2$  is a function of unknown parameters. However, the possibility arises of estimating  $D^2$  from the  $x_{1i}$  ( $i = 1, 2, \dots, n_1$ ) and the  $x_{2j}$  ( $j = 1, 2, \dots, n_2$ ). But substituting some estimator  $\hat{D}^2$  for  $D^2$  into equation 1.29 still leaves the approximated  $H'(k)$  in a complicated and unsatisfactory form. Therefore this avenue of approach is abandoned.

Consider next the approximation of  $H'(k)$  by a Taylor's series expansion of  $H'(k)$  about  $k = 0$ . Although it is suspected that zero is not necessarily the optimal discrimination point, it is anticipated that the optimal discrimination point is relatively "close" to zero. This expected "closeness" justifies the use of the Taylor's series expansion.

Taking the derivative of  $H(k)$  with respect to  $k$  and setting  $H'(k)$  equal to zero gives

$$(1.30) \quad H'(k_0) = 0 \doteq H'(0) + k_0 H''(0),$$

where  $k_0$  denotes the value of  $k$  which minimizes  $H(k)$ . Restating equation 1.30 in terms of  $f(k)$  and  $g(k)$  gives

$$(1.31) \quad f'(0) + g'(0) + k_0[f''(0) + g''(0)] \doteq 0.$$

From equation 1.27, it is easily seen that  $f'(0) = 0$ . The original definition of  $f(k)$  and  $g(k)$  breaks  $H(k)$  (as given in equation 1.24) into leading terms and first order (with respect to  $n_1^{-1}$ ,  $n_2^{-1}$  and  $(n_1 + n_2 - 2)^{-1}$ ) terms. Since  $k$  is assumed to be relatively "close" to zero, it follows that  $k_0[g''(0)]$  is of a higher order than the other terms in equation 1.31, and hence may be omitted. Thus the solution,  $k_0$ , to the discrimination point problem is given by

$$(1.32) \quad k_0 = -\frac{g'(0)}{f''(0)}.$$

Setting  $k$  equal to zero in equation 1.28 gives

$$(1.33) \quad g'(0) = [(2n_1 D^3)^{-1} (3-p-[6-p] \frac{D^2}{4} + \frac{D^4}{16} + p \frac{D^2}{2}) \\ + (2n_2 D^3)^{-1} (3-p-D^2 + [6-p] \frac{D^2}{4} + \frac{D^4}{16})] \phi(-\frac{D}{2}) \\ + [(2n_1 D^3)^{-1} (-[3-p] + D^2 - [6-p] \frac{D^2}{4} - \frac{D^4}{16}) \\ + (2n_2 D^3)^{-1} (-[3-p] + [6-p] \frac{D^2}{4} - \frac{D^4}{16} - p \frac{D^2}{2})] \phi(-\frac{D}{2}).$$

Collecting terms of equation 1.33 and simplifying gives

$$(1.34) \quad g'(0) = [(2n_1 D)^{-1}(p-2) - (2n_2 D)^{-1}(p-2)]\phi\left(\frac{D}{2}\right).$$

Taking the derivative with respect to  $k$  of each side of equation 1.27 gives

$$(1.35) \quad f''(k) = -D^{-2}\left(\frac{k}{D} - \frac{D}{2}\right)\phi\left(\frac{k}{D} - \frac{D}{2}\right) + D^{-2}\left(\frac{k}{D} + \frac{D}{2}\right)\phi\left(\frac{k}{D} + \frac{D}{2}\right).$$

Evaluating equation 1.35 at  $k = 0$  gives

$$(1.36) \quad f''(0) = D^{-1}\phi\left(\frac{D}{2}\right).$$

Thus from equations 1.32, 1.34, and 1.36, it follows that

$$(1.37) \quad k_0 = -(n_1^{-1} + n_2^{-1})\left(\frac{p-2}{2}\right).$$

The desirable classification procedure given by procedure 1.20 when  $k = k_0$  therefore is given by

$$(1.38) \quad \begin{aligned} &\text{Classify } X \text{ as belonging to } \pi_1 \text{ whenever } W \geq -(n_1^{-1} - n_2^{-1})\left(\frac{p-2}{2}\right); \\ &\text{classify } X \text{ as belonging to } \pi_2 \text{ whenever } W < -(n_1^{-1} - n_2^{-1})\left(\frac{p-2}{2}\right). \end{aligned}$$

#### Probabilities of Misclassification

Since the classification procedure given by procedure 1.38 is appropriate only when the parameter values are unknown, the probabilities of misclassification which are relevant are the conditional (on  $\bar{x}_1$ ,  $\bar{x}_2$  and  $S$ ) probabilities of misclassification,  $P_1$  and  $P_2$  (defined by equations 1.15), and the unconditional probabilities of misclassification,  $P_1^*$  and  $P_2^*$  (defined by equations 1.14). To avoid confusion, each of these probabilities will henceforth be written in general as a function of  $k$  and in

particular as a function of either zero or  $k_0 = -(n_1^{-1} - n_2^{-1})(\frac{p-2}{2})$ .

The conditional probabilities of misclassification under procedure 1.38, that is  $P_1(k_0)$  and  $P_2(k_0)$ , can be written more precisely as

$$(1.39) \quad P_1(k_0) = \Pr\{W < -(n_1^{-1} - n_2^{-1})(\frac{p-2}{2}) \mid \bar{x}_1, \bar{x}_2, S, X \in \pi_1\}, \text{ and}$$

$$P_2(k_0) = \Pr\{W \geq -(n_1^{-1} - n_2^{-1})(\frac{p-2}{2}) \mid \bar{x}_1, \bar{x}_2, S, X \in \pi_2\}.$$

Again noting that the conditional distribution of  $W$  given  $\bar{x}_1, \bar{x}_2$  and  $S$  is

$$N([\mu_1 - \frac{1}{2}(\bar{x}_1 + \bar{x}_2)]'S^{-1}[\bar{x}_1 - \bar{x}_2], [\bar{x}_1 - \bar{x}_2]'S^{-1}\Sigma S^{-1}[\bar{x}_1 - \bar{x}_2]) \text{ or}$$

$$N([\mu_2 - \frac{1}{2}(\bar{x}_1 + \bar{x}_2)]'S^{-1}[\bar{x}_1 - \bar{x}_2], [\bar{x}_1 - \bar{x}_2]'S^{-1}\Sigma S^{-1}[\bar{x}_1 - \bar{x}_2])$$

as  $X$  comes from  $\pi_1$  or  $\pi_2$ , equations 1.39 can be written

$$(1.40) \quad P_1(k_0) = \Phi \left[ \frac{-(n_1^{-1} - n_2^{-1})(\frac{p-2}{2}) - (\mu_1 - \frac{1}{2}[\bar{x}_1 + \bar{x}_2])'S^{-1}(\bar{x}_1 - \bar{x}_2)}{[(\bar{x}_1 - \bar{x}_2)'S^{-1}\Sigma S^{-1}(\bar{x}_1 - \bar{x}_2)]^{1/2}} \right]$$

$$P_2(k_0) = \Phi \left[ \frac{(n_1^{-1} - n_2^{-1})(\frac{p-2}{2}) + (\mu_2 - \frac{1}{2}[\bar{x}_1 + \bar{x}_2])'S^{-1}(\bar{x}_1 - \bar{x}_2)}{[(\bar{x}_1 - \bar{x}_2)'S^{-1}\Sigma S^{-1}(\bar{x}_1 - \bar{x}_2)]^{1/2}} \right].$$

The unconditional probabilities of misclassification,  $P_1^*(k_0)$  and  $P_2^*(k_0)$  (using the definitions in equations 1.14) can be written

$$(1.41) \quad P_1^*(k_0) = \Pr\{W < -(n_1^{-1} - n_2^{-1})(\frac{p-2}{2}) \mid X \in \pi_1\}, \text{ and}$$

$$P_2^*(k_0) = \Pr\{W \geq -(n_1^{-1} - n_2^{-1})(\frac{p-2}{2}) \mid X \in \pi_2\}.$$

Since the distribution of  $W$  is intractable, it is not easy to obtain expressions for  $P_1^*(k_0)$  and  $P_2^*(k_0)$  in terms of the parameters  $\pi_1$  and  $\pi_2$ . It

is noted, however, that  $P_1(k_0)$  and  $P_2(k_0)$  are unbiased estimators for  $P_1^*(k_0)$  and  $P_2^*(k_0)$ , respectively.



## COMPARISONS AND SUMMARY

## Numerical Evidence

To evaluate the performances of the two classification procedures, that using zero as the discrimination point and that using  $k_0$ , the basis of comparison is  $H(k)$  as defined by equation 1.21. Although the Taylor's series expansion as given by equation 1.24 might be used to evaluate the reduction,  $[H(0) - H(k_0)]$ , of  $H(k)$  under procedure 1.38, two objections are immediately apparent. The first, that the approximation of  $H(k)$  by a truncated Taylor's series expansion is insufficiently exact, might (conceptually) be dealt with by including terms of sufficiently high order. (However, the algebraic manipulations required to obtain even the second and certainly the third order terms are horrendous; terms of yet higher order would severely tax the most patient researcher.) The second objection, as even a cursory glance at  $H(k)$  suggests, is that when an expression for  $[H(0) - H(k_0)]$  is obtained, meaningful conclusions cannot be drawn from it. Almost nothing can be said of the expression without substituting specific values for the various parameters and for the sample sizes.

Hence, a Monte Carlo sampling experiment was conducted to determine the degree of improvement (in terms of  $H(k)$ ) of procedure 1.38 over procedure 1.7. Since the linear discriminant function  $W$  is invariant under any scale or location transformation, the distributions of

$\pi_1$  and  $\pi_2$  were assumed (without loss of generality) to be  $p$ -dimensional normal with  $\mu_1' = (0, \dots, 0)$ ,  $\mu_2' = (D, 0, \dots, 0)$  and  $\Sigma = I$  (the identity matrix). Since  $k_0 = 0$  when  $p = 2$ , only the values 3, 4, 8 and 20 were used for  $p$ ; and since  $k_0 = 0$  whenever  $n_1 = n_2$ , only unequal values of  $n_1$  and  $n_2$  were used. (Recalling that the numbering of the populations is arbitrary, it is necessary to consider here only the case  $n_1 < n_2$ .) The particular combinations of  $p$  and  $n_1$  and  $n_2$  are given in Table 1.

Table 1. Sample sizes and numbers of dimensions

p = 3		p = 4		p = 8		p = 20	
$n_1$	$n_2$	$n_1$	$n_2$	$n_1$	$n_2$	$n_1$	$n_2$
4	8	8	16	8	16	20	40
4	16	8	32	8	32	20	80
4	24	8	48	8	48		
10	20	20	40	20	40		
10	40	20	80	20	80		
10	60	20	120	20	120		

Six different values were used for the Mahalanobis distance. These values were chosen to correspond to particular values of the combined probability of misclassification under optimal circumstances (when all parameter values are known). Using equation 1.17, the values of  $D^2$

given in Table 2 were determined.

Table 2. Distances and corresponding values for  $P_1^{**} + P_2^{**}$

$D^2$	$P_1^{**} + P_2^{**}$
1.098	0.60
1.817	0.50
2.836	0.40
4.293	0.30
6.574	0.20
11.482	0.10

For each combination of parameters, random samples of sizes  $n_1$  and  $n_2$  were drawn from  $\pi_1$  and  $\pi_2$ . From these samples  $\bar{x}_1$ ,  $\bar{x}_2$  and  $S$  were computed.

Recall that  $P_1(k)$  and  $P_2(k)$  are unbiased estimators of  $P_1^*(k)$  and  $P_2^*(k)$ . Thus  $H(k)$  can be estimated by  $\hat{H}(k)$ , defined by

$$(1.42) \quad \hat{H}(k) = P_1(k) + P_2(k).$$

Using  $\bar{x}_1$ ,  $\bar{x}_2$  and  $S$ , both  $\hat{H}(0)$  and  $\hat{H}(-[n_1^{-1} - n_2^{-1}][\frac{p-2}{2}])$  were computed. Define by  $\Delta(p, n_1, n_2, D^2)_\ell$ ,

$$(1.43) \quad \Delta(p, n_1, n_2, D^2)_\ell = \hat{H}(0)_\ell - \hat{H}(-[n_1^{-1} - n_2^{-1}][\frac{p-2}{2}])_\ell \quad \text{for} \\ \ell = 1, 2, \dots, 100,$$

where  $\ell$  denotes the  $\ell^{\text{th}}$  repetition of the sampling experiment for the fixed parameters  $p, n_1, n_2$  and  $D^2$ . (For each combination of the parameters

$p, n_1, n_2$  and  $D^2$ , one hundred repetitions of the sampling experiment were made.) The criteria used to compare procedure 1.38 and procedure 1.7 are  $\bar{\Delta}(p, n_1, n_2, D^2)$  defined by

$$(1.44) \quad \bar{\Delta}(p, n_1, n_2, D^2) = \frac{1}{100} \sum_{\ell=1}^{100} \Delta(p, n_1, n_2, D^2)_{\ell},$$

and  $t(p, n_1, n_2, D^2)$  defined by

$$(1.45) \quad t(p, n_1, n_2, D^2) = \text{number } \{\Delta(p, n_1, n_2, D^2)_{\ell} < 0 \text{ for } \ell = 1, 2, \dots, 100\}.$$

In Tables 3, 4, 5 and 6, the values of  $\bar{\Delta}(p, n_1, n_2, D^2)$  are recorded with the corresponding values of  $t(p, n_1, n_2, D^2)$  given in parentheses underneath.

From Tables 3, 4, 5 and 6, four phenomena are readily observed. The first is that the value of  $t(p, n_1, n_2, D^2)$  exceeds 50 for only 7 of the 114 parameter combinations used. In other words, this numerical evidence suggests that with procedure 1.38 there is a smaller combined probability of misclassification. The second observation is that as the disparity of  $n_1$  and  $n_2$  increases, the performance of procedure 1.7 is increasingly inferior to that of procedure 1.38. Examination of either the values of  $\bar{\Delta}$  or the values of  $t$  leads to this result. Since the difference between  $k_0$  and zero increases as the ratio  $\frac{n_2}{n_1}$  increases, it might have been anticipated that the difference in the performance of the two procedures would also increase. Similarly, as  $p$  increases,  $k_0$

Table 3. Values for  $\bar{\Delta}(3, n_1, n_2, D^2)$  and  $t(3, n_1, n_2, D^2)$ 

$n_1, n_2$	$D^2=1.098$	$D^2=1.817$	$D^2=2.836$	$D^2=4.293$	$D^2=6.574$	$D^2=11.482$
4, 8	.00059602 (37)	-.00012391 (47)	.00008091 (40)	.00055602 (37)	-.00021849 (59)	-.00008744 (54)
4, 16	.00050471 (36)	.00100230 (38)	-.00008898 (43)	.00122736 (33)	.00022482 (41)	-.00000655 (47)
4, 24	.00043034 (35)	.00202128 (30)	-.00073648 (37)	.00073318 (39)	.00043169 (45)	.00020030 (43)
10, 20	-.00006664 (43)	.00008413 (41)	.00015496 (45)	-.00005052 (46)	.00003280 (51)	.00003783 (51)
10, 40	.00037113 (31)	-.00000574 (42)	-.00010430 (47)	-.00002720 (46)	.00010814 (45)	.00006388 (39)
10, 60	.00019707 (35)	.00017836 (30)	.00003406 (39)	.00013912 (41)	-.00002739 (50)	.00004849 (42)

Table 4. Values for  $\bar{\Delta}(4, n_1, n_2, D^2)$  and  $t(3, n_1, n_2, D^2)$

$n_1, n_2$	$D^2=1.098$	$D^2=1.817$	$D^2=2.836$	$D^2=4.293$	$D^2=6.574$	$D^2=11.482$
8, 16	.00014373 (45)	.00045703 (41)	.00041372 (36)	.00046501 (45)	-.00004177 (52)	.00005083 (47)
8, 32	.00099086 (31)	.00117291 (34)	-.00054964 (47)	.00027542 (39)	.00025622 (42)	-.00011253 (48)
8, 48	.00151903 (31)	.00080418 (44)	.00110629 (38)	.00043181 (40)	.00085485 (35)	.00013077 (45)
20, 40	.00006370 (46)	-.00005782 (46)	.00006687 (47)	.00003941 (47)	.00011304 (40)	-.00001400 (53)
20, 80	-.00021611 (49)	.00017794 (41)	.00035265 (36)	.00006201 (43)	.00012257 (40)	.00003691 (42)
20, 120	.00008079 (45)	.00054317 (31)	.00011801 (42)	.00022996 (39)	.00000728 (45)	.00006857 (40)

Table 5. Values for  $\bar{\Delta}(8, n_1, n_2, D^2)$  and  $t(8, n_1, n_2, D^2)$ 

$n_1, n_2$	$D^2=1.098$	$D^2=1.817$	$D^2=2.836$	$D^2=4.293$	$D^2=6.574$	$D^2=11.482$
8, 16	.00066258 (35)	.00056364 (41)	.00125513 (37)	.00110956 (38)	.00027200 (44)	-.00005167 (54)
8, 32	.00309417 (23)	.00429165 (24)	.00168518 (34)	.00184777 (33)	nc <sup>a</sup>	nc
8, 48	.00463264 (27)	.00628243 (21)	.00419094 (31)	.00360128 (31)	.00349234 (29)	.00118280 (37)
20, 40	.00046681 (34)	.00058087 (42)	.00051808 (37)	.00019562 (42)	.00020009 (46)	.00019649 (41)
20, 80	.00115990 (35)	.00163543 (33)	.00098799 (33)	.00048899 (41)	.00043931 (46)	.00036609 (38)
20, 120	.00117947 (27)	.00149078 (30)	.00074024 (39)	.00089983 (35)	.00062498 (35)	.00007181 (47)

<sup>a</sup>Not computed.

Table 6. Values of  $\bar{\Delta}(20, n_1, n_2, D^2)$  and  $t(20, n_1, n_2, D^2)$ 

$n_1, n_2$	$D^2=1.098$	$D^2=1.817$	$D^2=2.836$	$D^2=4.293$
20, 40	.00121017 (25)	.00153557 (29)	.00110834 (31)	.00102615 (35)
20, 80	.00580815 ( 7)	.00453632 (17)	.00556024 (12)	.00446560 (20)

differs more from zero; and a more marked difference between the performances of the two procedures might be expected. This conclusion also is borne out by examination of the tabled values of either  $\bar{\Delta}$  or  $t$ .

When  $D^2$  is varied, the pattern of behavior of  $\bar{\Delta}$  and  $t$  is not as regular as when  $\frac{n_2}{n_1}$  or  $p$  takes on different values. In general, however,  $\bar{\Delta}$  decreases as  $D^2$  is increased. This response to increases in  $D^2$  seems reasonable since  $[P_1^{**} + P_2^{**}]$  also decreases as  $D^2$  is increased. It is interesting to note that despite the behavior of  $\bar{\Delta}$ , both  $\frac{\bar{\Delta}}{P_1^{**} + P_2^{**}}$  and  $t$  increase as  $D^2$  is increased. The explanation of this phenomenon would seem to lie in the fact that when  $D^2$  is large, only the tails of the distributions of  $\pi_1$  and  $\pi_2$  overlap. Hence,  $P_1(k)$  and  $P_2(k)$  are estimates of "tail probabilities." The ratios

$\frac{P_1(k)}{P_1^{**}(k)}$  and  $\frac{P_2(k)}{P_2^{**}(k)}$ , also  $\frac{P_1(k)}{P_1^{**}(k)}$  and  $\frac{P_2(k)}{P_2^{**}(k)}$ , as functions of tail



probabilities, are quite sensitive to errors in estimation of the parameters of  $\pi_1$  and  $\pi_2$ . Thus (in the case of normal populations), poor estimates of either  $\mu_1$  and  $\mu_2$  or  $\Sigma$  are apt to produce more pronounced deviations of these functions relative to the "true" values in the tails of the distribution than nearer the means. Hence the slightly more erratic behavior of  $\bar{\Delta}$  and  $t$  for large  $D^2$  may be attributed not to the behavior of  $[H(0) - H(k)]$ , but rather to the inaccurate estimation of  $\mu_1, \mu_2$  and  $\Sigma$ .

The last observation to be made about  $\bar{\Delta}$  is that relative even to  $[P_1^{**} + P_2^{**}]$ ,  $\bar{\Delta}$  is in almost all cases so small as to be negligible. (Recall that  $[P_1^* + P_2^*]$  exceeds  $[P_1^{**} + P_2^{**}]$ , so comparison of  $\bar{\Delta}$  with  $[P_1^{**} + P_2^{**}]$  is optimistic relative to procedure 1.38.) A quick glance at any one of Tables 3, 4, 5 and 6 together with Table 2 confirms this.

### Conclusions

The problem treated in this part of the dissertation is that of choosing an optimal discrimination point for the two-population (multivariate normal) classification procedure. It has been demonstrated that the usual discrimination point, zero, is not always an optimal choice; and an alternative discrimination point,  $k_0 = -(n_1^{-1} - n_2^{-1})(\frac{p-2}{2})$ , has been proposed. The classification procedure using  $k_0$  has several attributes which recommend it. The value of  $k_0$  is easily determined without recourse to a machine of any type; and it has been shown that the procedure using  $k_0$

is a more desirable procedure than that using zero as the discrimination point. Unfortunately, the degree of improvement is so slight as to make the two procedures' performances comparable for all practical purposes. On the other hand, it is perhaps reassuring to be able to demonstrate that the commonly used procedure performs in so nearly optimal a manner.

PART II. ESTIMATION OF THE PROBABILITIES OF MISCLASSIFICATION IN  
THE UNIVARIATE NORMAL CASE

## PROBABILITIES OF MISCLASSIFICATION AND THEIR ESTIMATORS

### Three Distinct Probabilities of Misclassification

The probability of misclassification inherent in the use of a linear discriminant function is not necessarily known to the experimenter using such a function. Various estimators which may be calculated from the sample used to generate the sample discriminant function have been proposed. In this part of the dissertation, discussion is restricted to the case where each of the distributions is univariate normal and they are assumed to have common variance.

Let  $x_{1i}$  ( $i = 1, 2, \dots, n_1$ ) and  $x_{2j}$  ( $j = 1, 2, \dots, n_2$ ) denote two independent random samples from normal populations  $\pi_1$  and  $\pi_2$  having means  $\mu_1$  and  $\mu_2$  ( $\mu_1 < \mu_2$ ) and variance  $\sigma^2$ . Let  $X$  be a subsequently and independently (of the  $x_{1i}$  and of the  $x_{2j}$ ) drawn observation from either  $\pi_1$  or  $\pi_2$ . To classify  $X$  as belonging to  $\pi_1$  or  $\pi_2$ , the linear discriminant function,  $W$ , may be used. It takes the form

$$(2.1) \quad W = [X - \frac{1}{2}(\bar{x}_1 + \bar{x}_2)](\bar{x}_1 - \bar{x}_2)/\sigma^2 \quad \text{when } \sigma^2 \text{ is known}$$

$$= [X - \frac{1}{2}(\bar{x}_1 + \bar{x}_2)](\bar{x}_1 - \bar{x}_2)/s^2 \quad \text{when } \sigma^2 \text{ is unknown;}$$

$$\text{where } \bar{x}_1 = n_1^{-1} \sum_{i=1}^{n_1} x_{1i}, \quad \bar{x}_2 = n_2^{-1} \sum_{j=1}^{n_2} x_{2j}, \text{ and } s^2 =$$

$$(n_1 + n_2 - 2)^{-1} \left[ \sum_{i=1}^{n_1} (x_{1i} - \bar{x}_1)^2 + \sum_{j=1}^{n_2} (x_{2j} - \bar{x}_2)^2 \right].$$

Commonly,  $X$  is classified as belonging to  $\pi_1$  or  $\pi_2$  as the observed value of  $W$  is positive or negative. Thus the classification procedure may be written as

(2.2) Classify  $X$  as belonging to  $\pi_1$  if  $X < \frac{1}{2}(\bar{x}_1 + \bar{x}_2)$  and  $\bar{x}_1 < \bar{x}_2$  or if  $X > \frac{1}{2}(\bar{x}_1 + \bar{x}_2)$  and  $\bar{x}_1 > \bar{x}_2$ ; classify  $X$  as belonging to  $\pi_2$  otherwise.

Two distinct probabilities of misclassification, conditional (on  $\bar{x}_1$  and  $\bar{x}_2$ ) and unconditional, are relevant. First, the conditional probability that  $X$  be misclassified as belonging to  $\pi_1$  when  $X$  is from  $\pi_2$  is given by

$$(2.3) \quad P_2 = \Pr \left\{ X < \frac{1}{2}(\bar{x}_1 + \bar{x}_2) \mid \bar{x}_1, \bar{x}_2, X \in \pi_2 \right\} \text{ when } \bar{x}_1 < \bar{x}_2$$

$$= \Pr \left\{ X > \frac{1}{2}(\bar{x}_1 + \bar{x}_2) \mid \bar{x}_1, \bar{x}_2, X \in \pi_2 \right\} \text{ when } \bar{x}_1 > \bar{x}_2 .$$

An alternative form of equation 2.3 is

$$(2.4) \quad P_2 = \Phi \left( \left[ \frac{1}{2}(\bar{x}_1 + \bar{x}_2) - \mu_2 \right] / \sigma \right) \quad \text{when } \bar{x}_1 < \bar{x}_2$$

$$= 1 - \Phi \left( \left[ \frac{1}{2}(\bar{x}_1 + \bar{x}_2) - \mu_2 \right] / \sigma \right) \quad \text{when } \bar{x}_1 > \bar{x}_2 ,$$

where  $\Phi$  is the cumulative distribution function of a standard normal random variable. Second, the unconditional probability of misclassification is

$$(2.5) \quad P_2^* = \Pr \left\{ X < \frac{1}{2}(\bar{x}_1 + \bar{x}_2), \bar{x}_1 < \bar{x}_2 \mid X \in \pi_2 \right\}$$

$$+ \Pr \left\{ X > \frac{1}{2}(\bar{x}_1 + \bar{x}_2), \bar{x}_1 > \bar{x}_2 \mid X \in \pi_2 \right\},$$

which is, by definition, the expectation (with respect to  $\bar{x}_1$  and  $\bar{x}_2$ ) of  $P_2$ . It may be noted that since the numbering of the populations is arbitrary, the problem treated here is symmetric; and hence only the various errors of the second kind (classifying  $X$  as belonging to  $\pi_1$  when  $X$  comes from  $\pi_2$ ) are considered.

A third probability of misclassification is of interest for purposes of comparison. If all the parameters,  $\mu_1$ ,  $\mu_2$  ( $\mu_1 < \mu_2$ ) and  $\sigma^2$  should be known, the following classification procedure might be used

$$(2.6) \quad \begin{aligned} &\text{Classify } X \text{ as belonging to } \pi_1 \text{ if } X < \frac{1}{2}(\mu_1 + \mu_2); \\ &\text{classify } X \text{ as belonging to } \pi_2 \text{ if } X > \frac{1}{2}(\mu_1 + \mu_2) \end{aligned}$$

instead of the procedure 2.2. This new procedure leads to the probability of misclassification

$$(2.7) \quad P_2^{**} = \Phi\left(\frac{1}{2}[\mu_1 - \mu_2]/\sigma\right).$$

This represents the optimal situation in some sense; and both  $P_2$  and  $P_2^*$  are expected to be greater than  $P_2^{**}$  because of the lack of information on  $\mu_1$  and  $\mu_2$ .

The problem considered here is the estimation of the conditional probability,  $P_2$ . It is noted that  $P_2$  is a random variable since it is a function of  $\bar{x}_1$  and  $\bar{x}_2$ . Of the several authors (especially John (1961), Okamoto (1963), Hills (1966), Geisser (1967), Lachenbruch and Mickey (1968), and Sorum (1968)) who have treated the probability of misclassification problem, Hills, Lachenbruch and Mickey, and

Sorum have particularly addressed themselves to the problems of estimating  $P_2$  and of evaluating the estimators derived. Hills gave a general formulation of the classification problem when two populations are involved. He obtained some general analytical results about  $P_2$  and its estimators. By assuming particular distributions (including normal) and using numerical examples, Hills obtained more precise results. Lachenbruch and Mickey compared several estimators of  $P_2$  using a Monte Carlo sampling experiment and obtained fairly conclusive results. Sorum made an extensive analytical investigation of this problem for the cases of univariate and multivariate normal distributions with known variance and known covariance matrix, respectively. She used the conditional mean square error as the criterion for comparison of estimators of  $P_2$ . This criterion failed to confirm the findings of Lachenbruch and Mickey because of inadequate discrimination among estimators. The criterion of unconditional mean square error used in this dissertation both seems a more meaningful measure of performance and provides clearer discrimination among the estimators, giving the support of analytical results for the univariate case to the numerical evidence of Lachenbruch and Mickey.

#### Estimators of the Probabilities of Misclassification

Of the eight estimators of  $P_2$  (the conditional probability of misclassification) to be considered, only the first two do not require any

distribution assumptions about  $\pi_1$  and  $\pi_2$ ; the others rely on the assumption of the normality of  $\pi_1$  and  $\pi_2$ .

The reclassification estimator,  $P_R$ , suggested by Smith (1947) is one of the classical estimators of  $P_2$ . To compute  $P_R$ , the discrimination procedure 2.2 must be formulated from the  $n_1$  observations from  $\pi_1$  and the  $n_2$  observations from  $\pi_2$ . Then each of the  $n_2$  observations from  $\pi_2$  is classified according to the procedure. The estimator,  $P_R$ , is the proportion of the  $n_2$  observations misclassified by the procedure as belonging to  $\pi_1$ .

The "jackknife" estimator,  $P_U$ , was proposed by Lachenbruch and Mickey (1968) as "method U." To compute the value of  $P_U$ , it is necessary to make all possible  $(n_2 - 1, 1)$  "splits" of the sample from  $\pi_2$ . For each possible split, a discrimination procedure 2.2 is formulated from  $n_1$  and  $n_2 - 1$  observations on  $\pi_1$  and  $\pi_2$ , respectively. Then the remaining observation from  $\pi_2$  is classified according to this procedure. The estimator,  $P_U$ , is the proportion of the  $n_2$  observations from  $\pi_2$  which are misclassified as belonging to  $\pi_1$ .

Another classical estimator for  $P_2$  is  $P_D$ , which is obtained by substituting the usual sample estimates into the expression for  $P_2$  given by equation 2.4. Hence, if  $\sigma^2$  is known,

$$\begin{aligned} (2.8) \quad P_D &= \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/\sigma\right] \text{ if } \bar{x}_1 < \bar{x}_2 \\ &= 1 - \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/\sigma\right] \text{ if } \bar{x}_1 > \bar{x}_2 ; \end{aligned}$$



if  $\sigma^2$  is unknown

$$(2.9) \quad P_D = \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/s\right] \text{ if } \bar{x}_1 < \bar{x}_2 \\ = 1 - \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/s\right] \text{ if } \bar{x}_1 > \bar{x}_2 .$$

To define the estimators  $P_O^*$  and  $P_{OS}^*$ , the asymptotic expansion of  $P_2^*$  due to Okamoto (1963) is used, giving

$$(2.10) \quad P_2^* = \Phi\left[\frac{1}{2}(\mu_1 - \mu_2)/\sigma\right] - \frac{1}{16}[(\mu_1 - \mu_2)/\sigma](n_1^{-1} + n_2^{-1})\phi\left[\frac{1}{2}(\mu_1 - \mu_2)/\sigma\right] + O_2$$

where  $O_2$  denotes the second order terms of  $(n_1^{-1}, n_2^{-1}, [n_1 + n_2 - 2]^{-1})$ .

Although not really estimates of  $P_2$ , but rather of  $P_2^*$ , the estimators  $P_O^*$  and  $P_{OS}^*$  (corresponding to the "O" and "OS" methods of Lachenbruch and Mickey) might still be useful and hence are included in this discussion. Substitution of the usual estimators for  $\mu_1$  and  $\mu_2$  (and for  $\sigma^2$  when  $\sigma^2$  is unknown) gives  $P_O^*$ . Then when  $\sigma^2$  is known

$$(2.11) \quad P_O^* = \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/\sigma\right] - \frac{1}{16}[(\bar{x}_1 - \bar{x}_2)/\sigma][n_1^{-1} + n_2^{-1}]\phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/\sigma\right];$$

and when  $\sigma^2$  is unknown,

$$(2.12) \quad P_O^* = \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/s\right] - \frac{1}{16}[(\bar{x}_1 - \bar{x}_2)/s][n_1^{-1} + n_2^{-1}]\phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/s\right] .$$

When  $\sigma^2$  is unknown, substitution into expression 2.10 of the square root of an unbiased estimator for  $(\mu_1 - \mu_2)^2/\sigma^2$  gives  $P_{OS}^*$ . Thus,

$$(2.13) \quad P_{OS}^* = \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)(n_1 + n_2 - 4)^{1/2}/s(n_1 + n_2 - 2)^{1/2}\right] \\ - \frac{1}{16}[(\bar{x}_1 - \bar{x}_2)(n_1 + n_2 - 4)^{1/2}/s(n_1 + n_2 - 2)^{1/2}][n_1^{-1} + n_2^{-1}] \\ \cdot \phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)(n_1 + n_2 - 4)^{1/2}/s(n_1 + n_2 - 2)^{1/2}\right] .$$

Another estimator for the case when  $\sigma^2$  is unknown is  $P_{DS}^{**}$ .

Substitution of the square root of the unbiased estimator for

$(\mu_1 - \mu_2)^2/\sigma^2$  into expression 2.7 gives the "DS" method of

Lachin (1966) and Mickey;

$$(2.14) \quad P_{DS}^{**} = \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)(n_1 + n_2 - 4)^{1/2}/s(n_1 + n_2 - 2)^{1/2}\right].$$

Bayesian arguments suggest  $P_G$  and  $P_S$ , estimators constructed by Geisser (1967) and Sorum (1968), respectively.

$$(2.15) \quad P_G = \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/\sigma(1 + n_2^{-1})^{1/2}\right] \text{ when } \sigma^2 \text{ is known;}$$

and when  $\sigma^2$  is unknown,

$$(2.16) \quad P_G = \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/s(1 + n_2^{-1})^{1/2}\right];$$

$$(2.17) \quad P_S = \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/\sigma(1 + \frac{1}{2}n_2^{-1})^{1/2}\right] \text{ when } \sigma^2 \text{ is known,}$$

and when  $\sigma^2$  is unknown,

$$(2.18) \quad P_S = \Phi\left[\frac{1}{2}(\bar{x}_1 - \bar{x}_2)/s(1 + \frac{1}{2}n_2^{-1})^{1/2}\right].$$

It is noted that since the event  $\bar{x}_1 > \bar{x}_2$  has probability of the order  $o(n_1^{-1}, n_2^{-1})^k$  for any  $k$  as  $n_1, n_2 \rightarrow \infty$  because of the assumption  $\mu_1 < \mu_2$ , equations 2.2, 2.4, 2.5, 2.8 and 2.9 can be rewritten as

$$(2.19) \quad \text{Classify } X \text{ as belonging to } \pi_1 \text{ if } X < \frac{1}{2}(\bar{x}_1 + \bar{x}_2);$$

classify  $X$  as belonging to  $\pi_2$  otherwise;

$$(2.20) \quad P_2 \doteq ([\frac{1}{2}(\bar{x}_1 + \bar{x}_2) - \mu_2]/\sigma);$$

$$(2.21) \quad P_2^* \doteq \Pr \{X < \frac{1}{2} (\bar{x}_1 + \bar{x}_2) \mid X \in \pi_2\}; \text{ and}$$

$$(2.22) \quad P_D \doteq \Phi[\frac{1}{2} (\bar{x}_1 - \bar{x}_2)/\sigma] \text{ when } \sigma^2 \text{ is known;}$$

$$(2.23) \quad P_D \doteq \Phi[\frac{1}{2} (\bar{x}_1 - \bar{x}_2)/s] \text{ when } \sigma^2 \text{ is unknown.}$$

(Since the terms omitted in equations 2.20, 2.21, 2.23 and 2.24 are negligible, the notation of approximation is not used henceforth.)

The estimators in equations 2.22 and 2.23 can also be obtained by the substitution of the sample estimates into equation 2.7. The expansion 2.11 actually follows easily from 2.21.

# MEAN SQUARE ERRORS FOR THE $\sigma^2$ KNOWN CASE

## Mean Square Errors for Estimators Requiring No Distribution Assumptions

The unconditional mean square errors for the estimators  $P_R$  and  $P_U$  (which do not require any assumption about the distributions of  $\pi_1$  and  $\pi_2$ ) are derived below for the case when  $\sigma^2$  is known. The assumption that  $\sigma^2 = 1$  is made for convenience. This implies no loss of generality since the classification procedure is invariant under any scale transformation.

Consider a general estimator  $\hat{P}_2$  which includes  $P_R$  and  $P_U$  as special cases.

$$(2.24) \quad \hat{P}_2 = n_2^{-1} \sum_{j=1}^{n_2} \gamma_j$$

where  $\gamma_j = 1$  when  $X_{2j}$  is classified as belonging to  $\pi_1$

$= 0$  when  $X_{2j}$  is classified as belonging to  $\pi_2$

and  $X_{2j}$  is the  $j^{\text{th}}$  observation in the sample from  $\pi_2$ , for  $j = 1, 2, \dots, n_2$ .

$$(2.25) \quad E[(\hat{P}_2 - P_2)^2] = n_2^{-2} \sum_{j=1}^{n_2} E[\gamma_j^2] + 2n_2^{-2} \sum_{j < j'}^{n_2} E(\gamma_j \gamma_{j'}) \\ - 2n_2^{-1} \sum_{j=1}^{n_2} E(\gamma_j P_2) + E(P_2^2),$$

where  $E$  denotes expectation with respect to  $\bar{x}_1$ ,  $\bar{x}_2$  and  $\gamma_j$ . Since  $P_2^2$  is not a function of the  $\gamma_j$ ,  $E(P_2^2)$  denotes the expectation of  $P_2^2$  with respect to  $\bar{x}_1$  and  $\bar{x}_2$ .

To evaluate  $E(P_2^2)$ , first define  $\xi_0$  by

$$(2.26) \quad \xi_0 = \frac{1}{2} (\bar{x}_1 + \bar{x}_2) - \mu_2;$$

the  $\xi_0$  follows a normal distribution with mean  $\frac{1}{2}(\mu_1 - \mu_2)$  and variance  $\frac{1}{4}(n_1^{-1} + n_2^{-1})$ . From expression 2.20 it follows that

$$(2.27) \quad P_2 = \Phi(\xi_0)$$

(Recall that the terms omitted in equation 2.27 are negligible and that the notation of approximation was dropped after equations 2.20, 2.21, 2.23 and 2.24.)

Expanding each of  $P_2$  and  $P_2^2$  in a Taylor's series about the point  $\frac{1}{2}(\mu_1 - \mu_2)$  and taking the expectation with respect to  $\xi_0$  give

$$(2.28) \quad E(P_2) = \Phi_0 + \frac{1}{8}(n_1^{-1} + n_2^{-1})\Phi_2 + \frac{1}{128}(n_1^{-1} + n_2^{-1})^2\Phi_4 + O_3;$$

$$(2.29) \quad E(P_2^2) = \Phi_0^{(2)} + \frac{1}{8}(n_1^{-1} + n_2^{-1})\Phi_2^{(2)} + \frac{1}{128}(n_1^{-1} + n_2^{-1})^2\Phi_4^{(2)} + O_3,$$

$$\text{where } \Phi_k^{(r)} = \left. \frac{d^k [\Phi(t)]^r}{dt^k} \right|_{t = \frac{1}{2}(\mu_1 - \mu_2)} \quad \text{for } r = 1, 2; \quad k = 0, 2, 4, \text{ and}$$

$$\Phi_k^{(1)} = \Phi_k,$$

and where  $O_i$  denotes  $O(n_1^{-1}, n_2^{-1}, \text{ or } [n_1 + n_2 - 2]^{-1})^i$  for  $i = 1, 2, 3$ . (For realizations of the  $\Phi_k^{(r)}$  see the Appendix.) Equations 2.7, 2.10 and 2.27 show that to  $O_3$ , both  $P_2$  and  $P_2^*$  are larger than  $P_2^{**}$  in the sense of expectation.

Useful in evaluating the second term of expression 2.25 is the following lemma.

Lemma. If  $\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \sim N\left(\begin{pmatrix} \nu_1 \\ \nu_2 \end{pmatrix}; \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right)$ , and  $\rho$  is small, then

$$\begin{aligned} \Pr \{y_1 < 0, y_2 < 0\} &= \Phi(-\nu_1)\Phi(-\nu_2) + \rho\phi(-\nu_1)\phi(-\nu_2) \\ &\quad + \frac{1}{2}\rho^2\nu_1\nu_2\phi(-\nu_1)\phi(-\nu_2) + O(\rho^3). \end{aligned}$$

$$\begin{aligned} \text{Proof. } \Pr \{y_1 < 0, y_2 < 0\} &= (2\pi\sqrt{1-\rho^2})^{-1} \int_{-\infty}^0 \int_{-\infty}^0 \exp \left\{ -\frac{1}{2}[(y_1 - \nu_1)^2 + (y_2 - \nu_2)^2] / \right. \\ &\quad \left. (1 - \rho^2) \right\} \\ &\quad \cdot \exp \{ \rho(y_1 - \nu_1)(y_2 - \nu_2) / (1 - \rho^2) \} dy_1 dy_2 \end{aligned}$$

$$\begin{aligned} &= \sqrt{1-\rho^2} \int_{-\infty}^{-\nu_1(1-\rho^2)^{-1/2}} \int_{-\infty}^{-\nu_2(1-\rho^2)^{-1/2}} \phi(z_1)\phi(z_2)[1 + \rho z_1 z_2 + \\ &\quad \frac{1}{2}\rho^2 z_1^2 z_2^2 + O(\rho^3)] dz_1 dz_2 \end{aligned}$$

where  $z_1 = (1-\rho^2)^{-1/2}(y_1 - \nu_1)$  and  $z_2 = (1-\rho^2)^{-1/2}(y_2 - \nu_2)$ . Evaluation of the integral gives

$$\begin{aligned} \Pr \{y_1 < 0, y_2 < 0\} &= (1-\rho^2)^{1/2} \{ \Phi[-\nu_1(1-\rho^2)^{-1/2}] \Phi[-\nu_2(1-\rho^2)^{-1/2}] \\ &\quad + \rho \phi[-\nu_1(1-\rho^2)^{-1/2}] \phi[-\nu_2(1-\rho^2)^{-1/2}] + \frac{1}{2}\rho^2 (\Phi[-\nu_1(1-\rho^2)^{-1/2}] \\ &\quad + \nu_1(1-\rho^2)^{-1/2} \phi[-\nu_1(1-\rho^2)^{-1/2}]) \\ &\quad \cdot (\Phi[-\nu_2(1-\rho^2)^{-1/2}] + \nu_2(1-\rho^2)^{-1/2} \phi[-\nu_2(1-\rho^2)^{-1/2}]) \} + O(\rho^3). \end{aligned}$$

Expanding each of  $(1-\rho^2)^{1/2}$  and  $(1-\rho^2)^{-1/2}$  in a binomial series about 1, expanding each of  $\Phi[-\nu_i(1-\rho^2)^{-1/2}]$  and  $\phi[-\nu_i(1-\rho^2)^{-1/2}]$  in a Taylor's series about the point  $-\nu_i$  for  $i = 1, 2$  and simplifying complete the proof.

Consider now the estimator  $P_R$  and its unconditional mean square error as given by equations 2.24 and 2.25. Define  $\xi_j$  by

$$(2.30) \quad \xi_j = \frac{1}{2}(\bar{x}_1 + \bar{x}_2) - x_{2j} \quad \text{for } j = 1, 2, \dots, n_2;$$

then  $\xi_j$  follows a normal distribution with mean  $\frac{1}{2}(\mu_1 - \mu_2)$  and variance  $1 + \frac{1}{4}n_1^{-1} - \frac{3}{4}n_2^{-1}$ ; also  $\xi_j$  and  $\xi_{j'}$  have covariance  $\frac{1}{4}n_1^{-1} - \frac{3}{4}n_2^{-1}$  for  $j \neq j'$ . Since  $E(Y_j^2) = E(Y_j) = \Pr\{\xi_j > 0\}$ ,  $E(Y_j^2) = \Phi[\frac{1}{2}k(\mu_1 - \mu_2)]$  where  $k = (1 + \frac{1}{4}n_1^{-1} - \frac{3}{4}n_2^{-1})^{-1/2}$ . Using a binomial expansion of  $k$  about 1 and a Taylor's series expansion of  $\Phi[\frac{1}{2}k(\mu_1 - \mu_2)]$  about the point  $\frac{1}{2}(\mu_1 - \mu_2)$  results in

$$(2.31) \quad E(Y_j^2) = \Phi + \frac{1}{8}(n_1^{-1} - 3n_2^{-1})\Phi_2 + O_2 \quad \text{for any } j.$$

Since  $\begin{pmatrix} k\xi_j \\ k\xi_{j'} \end{pmatrix}$  is distributed according to  $N\left(\begin{pmatrix} \frac{1}{2}k(\mu_1 - \mu_2) \\ \frac{1}{2}k(\mu_1 - \mu_2) \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right)$

with  $\rho = \frac{1}{4}k(n_1^{-1} - 3n_2^{-1})$ , the lemma proved at the beginning of this section applies and

$$(2.32) \quad \begin{aligned} E(Y_j Y_{j'}) &= \Pr\{\xi_j > 0, \xi_{j'} > 0\} \\ &= \Phi^2[\frac{1}{2}k(\mu_1 - \mu_2)] + \rho\phi^2[\frac{1}{2}k(\mu_1 - \mu_2)] + \frac{1}{2}\rho^2[\frac{1}{2}k(\mu_1 - \mu_2)]^2\phi^2[\frac{1}{2}k(\mu_1 - \mu_2)] \\ &\quad + O_3 \end{aligned}$$

for any  $j \neq j'$ , where  $\phi$  is the density function of a standard normal variable. Using again a binomial expansion of  $k$  about 1 and Taylor's series expansions of  $\Phi[\frac{1}{2}k(\mu_1 - \mu_2)]$  and  $\phi[\frac{1}{2}k(\mu_1 - \mu_2)]$  about the point

$\frac{1}{2}(\mu_1 - \mu_2)$ , equation 2.32 can be rewritten as

$$(2.33) \quad E(\gamma_j \gamma_{j'}) = \Phi_0^2 + \frac{1}{8}(n_1^{-1} - 3n_2^{-1})\Phi_2^{(2)} + \frac{1}{128}(n_1^{-1} - 3n_2^{-1})^2 \Phi_4^{(2)} + O_3$$

for any  $j \neq j'$ .

Consider next  $E(\gamma_j P_2) = E_{\xi_0} [E(\gamma_j P_2 | \xi_0)] = E[\Phi(\xi_0) \cdot \Pr\{\xi_j > 0 | \xi_0\}]$ .

Since the conditional distribution of  $\xi_j | \xi_0$  is normal with mean

$$\frac{1}{2}(\mu_1 - \mu_2) + \beta[\xi_0 - \frac{1}{2}(\mu_1 - \mu_2)] \text{ and variance } \sigma_2^2 = 1 - n_2^{-1} + (n_1 + n_2)^{-1},$$

where  $\beta = (n_1^{-1} - n_2^{-1})/(n_1^{-1} + n_2^{-1})$ , it follows that  $E(\gamma_j P_2) = E[\psi(\xi_0)]$

where  $\psi(\xi_0) = \Phi(\xi_0) \Phi([\frac{1}{2}(\mu_1 - \mu_2) + \beta(\xi_0 - \frac{1}{2}[\mu_1 - \mu_2])]/\sigma_2)$ . Using

a development similar to the development of equation 2.29, results in

$$(2.34) \quad E(\gamma_j P_2) = \psi_0 + \frac{1}{8}(n_1^{-1} + n_2^{-1})\psi_2 + \frac{1}{128}(n_1^{-1} + n_2^{-1})^2 \psi_4 + O_3$$

$$\text{where } \psi_k = \left. \frac{d^k[\psi(t)]}{dt^k} \right|_{t=\frac{1}{2}(\mu_1 - \mu_2)} \quad \text{for } k = 0, 2, 4.$$

Straightforward calculation using binomial series, Taylor's series and

expectations with respect to  $\bar{x}_1$  and  $\bar{x}_2$  gives

$$(2.35) \quad E(\gamma_j P_2) = \Phi_0^{(2)} + \frac{1}{8}(n_1^{-1} - n_2^{-1})\Phi_2^{(2)} + \frac{1}{128}(n_1^{-2} - 5n_1^{-1}n_2^{-1} + 5n_2^{-2})\Phi_4^{(2)} \\ - \frac{1}{8}n_2^{-2}\Phi_2^{(2)} + O_3$$

$$\text{where } \phi_k^{(r)} = \left. \frac{d^k[\phi(t)]^r}{dt^k} \right|_{t=\frac{1}{2}(\mu_1 - \mu_2)} \quad \text{for } r = 1, 2 \text{ and } k = 0, 2.$$

By substituting expressions 2.29, 2.31, 2.33 and 2.35 into equation 2.25,

or, equivalently, into

$$(2.36) \quad E[(\hat{P}_2 - P_2)^2] = E(P_2^2) + n_2^{-1}E(\gamma_j^2) + (1 - n_2^{-1})E(\gamma_j \gamma_{j'}) - 2E(\gamma_j P_2),$$



the unconditional mean square error for  $P_R$  is obtained, and

$$(2.37) \quad E[(P_R - P_2)^2] = n_2^{-1} \Phi(1-\Phi) + \frac{1}{8} n_2^{-1} (n_1^{-1} - 3n_2^{-1}) (\Phi_2 - \Phi_2^{(2)}) \\ + \frac{1}{4} n_2^{-2} \phi_2^{(2)} + O_3 .$$

Consider next the estimator  $P_U$  and its unconditional mean square error given by equations 2.24 and 2.25. Following the same line of reasoning as that used to find the unconditional mean square error for  $P_R$  yields

$$(2.38) \quad E[(P_U - P_2)^2] = n_2^{-1} \Phi(1-\Phi) + \frac{1}{8} n_2^{-1} (n_1^{-1} + n_2^{-1}) (\Phi_2 - \Phi_2^{(2)}) \\ + \frac{1}{4} n_2^{-2} \phi_1^2 + O_3 .$$

#### Mean Square Errors for Estimators Requiring Distribution Assumptions

The following notation is convenient in obtaining the unconditional mean square errors of the estimators relying on the normality of  $\pi_1$  and  $\pi_2$ .

Letting

$$(2.39) \quad z_1 = \bar{x}_1 - \mu_1, \text{ and} \\ z_2 = \bar{x}_2 - \mu_2 ,$$

$z_1$  and  $z_2$  are independent normal random variables each with mean zero and with variances  $n_1^{-1}$  and  $n_2^{-1}$ , respectively. Denote by  $\zeta$  and  $\eta$  the quantities

$$(2.40) \quad \zeta = \frac{1}{2} (z_1 + z_2) \text{ and} \\ \eta = \frac{1}{2} (z_1 - z_2) .$$

Then  $P_2$  can be written

$$(2.41) \quad P_2 = \Phi\left[\frac{1}{2}(\mu_1 - \mu_2) + \zeta\right].$$

Recall that the terms omitted in equation (2.39) are arbitrarily small.

(See equation 2.20 and comment following equation 2.24.) Expanding

$P_2$  in a Taylor's series about the point  $\frac{1}{2}(\mu_1 - \mu_2)$  gives

$$(2.42) \quad P_2 \doteq \Phi_0 + \zeta \Phi_1 + \frac{1}{2} \zeta^2 \Phi_2 + \frac{1}{6} \zeta^3 \Phi_3 + \frac{1}{24} \zeta^4 \Phi_4$$

where the  $\Phi_k$  are as defined below equation 2.29 for  $k = 0, 1, 2, 3, 4$ .

Consider first the estimator  $P_D$ , which can be written

$$(2.43) \quad P_D = \Phi\left[\frac{1}{2}(\mu_1 - \mu_2) + \eta\right].$$

Expanding  $P_D$  in a Taylor's series about the point  $\frac{1}{2}(\mu_1 - \mu_2)$  gives an expansion analogous to the expression 2.42, but with  $\zeta$  replaced by  $\eta$ .

Thus, by taking the difference of these two expressions and squaring the result gives an approximate expression for  $(P_2 - P_D)^2$ , or

$$(2.44) \quad (P_2 - P_D)^2 \doteq (\zeta - \eta)^2 \Phi_1^2 + (\zeta - \eta)(\zeta^2 - \eta^2) \Phi_1 \Phi_2 + \frac{1}{3}(\zeta - \eta)(\zeta^3 - \eta^3) \Phi_1 \Phi_3 \\ + \frac{1}{4}(\zeta^2 - \eta^2)^2 \Phi_2^2.$$

Taking the expectation of equation 2.44 with respect to  $\zeta$  and  $\eta$  gives

$$(2.45) \quad E[(P_2 - P_D)^2] = n_2^{-1} \Phi_1^2 + \frac{1}{4}(n_1^{-1} n_2^{-1} + n_2^{-2}) \Phi_1 \Phi_3 + \frac{1}{4} n_1^{-1} n_2^{-1} \Phi_2^2 + O_3.$$

Consider next the estimator  $P_0^*$  which can be written

$$(2.46) \quad P_0^* = \Phi\left[\frac{1}{2}(\mu_1 - \mu_2) + \eta\right] + \frac{1}{8}(n_1^{-1} + n_2^{-1}) \Phi_2 \left[\frac{1}{2}(\mu_1 - \mu_2) + \eta\right].$$

Expanding each term of equation 2.46 in a Taylor's series about the point  $\frac{1}{2}(\mu_1 - \mu_2)$ , taking the difference of the resultant expression and equation

2.42 and squaring this difference give

$$\begin{aligned}
 (2.47) \quad (P_2 - P_0^*)^2 &= (\zeta - \eta)^2 \Phi_1^2 + (\zeta - \eta)(\zeta^2 - \eta^2) \Phi_1 \Phi_2 + \frac{1}{3}(\zeta - \eta)(\zeta^3 - \eta^3) \Phi_1 \Phi_3 \\
 &+ \frac{1}{4}(\zeta^2 - \eta^2)^2 \Phi_2^2 + \frac{1}{4}(n_1^{-1} + n_2^{-1})[(\zeta - \eta) \Phi_1 \Phi_2 + \frac{1}{2}(\zeta^2 - \eta^2) \Phi_2^2 \\
 &+ \frac{1}{6}(\zeta^3 - \eta^3) \Phi_2 \Phi_3 + \eta(\zeta - \eta) \Phi_1 \Phi_3 + \frac{1}{2}\eta(\zeta^2 - \eta^2) \Phi_2 \Phi_3 + \frac{1}{6}(\zeta^3 - \eta^3) \Phi_3^2] \\
 &+ \frac{1}{64}(n_1^{-1} + n_2^{-1})^2 \Phi_2^2.
 \end{aligned}$$

Taking the expectation of equation 2.47 with respect to  $\zeta$  and  $\eta$  gives

$$\begin{aligned}
 (2.48) \quad E[(P_2 - P_0^*)^2] &= n_2^{-1} \Phi_{10}^2 + \left( \frac{n_1^{-2} + n_2^{-2}}{64} + \frac{9n_1^{-1} n_2^{-1}}{32} \right) \Phi_{20}^2 + \\
 &+ \frac{3n_1^{-1} n_2^{-1} + 3n_2^{-2}}{8} \Phi_{10} \Phi_{30}.
 \end{aligned}$$

Finally, consider the estimators  $P_G$  and  $P_S$ . Each is a special case of the estimator  $\hat{P}_2$  given by

$$(2.49) \quad \hat{P}_2 = \Phi \left[ \left( \frac{1}{2} [\mu_1 - \mu_2] + \eta \right) (1 + a n_2^{-1})^{-1/2} \right]$$

where  $a$  takes the value 1 for  $P_G$  and the value  $\frac{1}{2}$  for  $P_S$ . Expanding

$(1 + a n_2^{-1})^{-1/2}$  in a binomial series about 1 and expanding

$\Phi \left[ \left( \frac{1}{2} [\mu_1 - \mu_2] + \eta \right) (1 + a n_2^{-1})^{-1/2} \right]$  in a Taylor's series about the point

$\frac{1}{2}(\mu_1 - \mu_2)$  give

$$\begin{aligned}
 (2.50) \quad \hat{P}_2 &= \Phi + \left[ \eta - \frac{1}{2}(\mu_1 - \mu_2) \left( \frac{1}{2} a n_2^{-1} - \frac{3}{8} a^2 n_2^{-2} \right) - \eta \left( \frac{1}{2} a n_2^{-1} - \frac{3}{8} a^2 n_2^{-2} \right) \right] \Phi_1 \\
 &+ \frac{1}{2} \left[ \frac{1}{16} (\mu_1 - \mu_2)^2 a^2 n_2^{-2} - \frac{1}{2} \eta (\mu_1 - \mu_2) + \eta^2 - \eta^3 a n_2^{-1} \right] \Phi_2 \\
 &+ \frac{1}{6} \left[ -\frac{3}{4} \eta^2 (\mu_1 - \mu_2) a n_2^{-1} + \eta^3 \left( 1 - \frac{1}{2} a n_2^{-1} \right) - \eta^4 a n_2^{-1} \right] \Phi_3.
 \end{aligned}$$

Taking the difference of equations 2.42 and 2.50, squaring it and taking

the expectation of the result yield

$$(2.51) \quad E[(P_2 - P_G)^2] = n_2^{-1} \Phi_1^2 + \frac{1}{4} (n_1^{-1} n_2^{-1} + n_2^{-2}) \Phi_1 \Phi_3 + \frac{1}{4} n_1^{-1} n_2^{-1} \Phi_2^2 \\ + n_2^{-2} \left[ \left( -\frac{1}{2} + \frac{1}{16} [\mu_1 - \mu_2]^2 \right) \Phi_1^2 + \frac{1}{4} (\mu_1 - \mu_2) \Phi_1 \Phi_2 \right] + O_3,$$

and

$$(2.52) \quad E[(P_2 - P_S)^2] = n_2^{-1} \Phi_1^2 + \frac{1}{4} (n_1^{-1} n_2^{-1} + n_2^{-2}) \Phi_1 \Phi_3 + \frac{1}{4} n_1^{-1} n_2^{-1} \Phi_2^2 \\ + n_2^{-2} \left[ \left( -\frac{1}{4} + \frac{1}{64} [\mu_1 - \mu_2]^2 \right) \Phi_1^2 + \frac{1}{8} (\mu_1 - \mu_2) \Phi_1 \Phi_2 \right] + O_3.$$

# MEAN SQUARE ERRORS FOR THE $\sigma^2$ UNKNOWN CASE

As was noted earlier in this part of the dissertation, only the estimators motivated by the assumption of normality of the underlying populations have different forms for the cases when  $\sigma^2$  is known and when  $\sigma^2$  is unknown. Hence the mean square errors for  $P_R$  and  $P_U$ , when  $\sigma^2$  is unknown, are the same as when  $\sigma^2$  is known and are given by equations 2.37 and 2.38, respectively.

The estimators motivated by the normality of  $\pi_1$  and  $\pi_2$  will now be considered. First note that the classification procedure 2.19 guarantees that  $P_2$  can still be written as

$$(2.52) \quad P_2 = \Phi\left[\frac{1}{2}(\mu_1 - \mu_2) + \zeta\right]$$

when  $\sigma^2$  is unknown. (Notation is as in equation 2.40.) The estimators

$P_D$ ,  $P_{DS}^{**}$ ,  $P_G$  and  $P_S$  can all be written in the general form

$$(2.53) \quad \hat{P}_2 = \Phi\left(\left[\frac{1}{2}(\mu_1 - \mu_2) + \eta\right]/[1 + \tau]^{1/2}[1 + \alpha]^{1/2}\right)$$

where  $\eta = \frac{1}{2}(z_1 - z_2)$ ,  $\tau = s^2 - 1$ , and  $\alpha$  takes on the values

$0$ ,  $2(n_1 + n_2 - 4)^{-1}$ ,  $n_2^{-1}$  and  $\frac{1}{2}n_2^{-1}$  for  $P_D$ ,  $P_{DS}^{**}$ ,  $P_G$  and  $P_S$ , respectively.

Consider the simplest case, that of  $P_D$ . As for the case when  $\sigma^2$  is known, equation 2.52 can be expanded in a simple Taylor's series about the point  $\frac{1}{2}(\mu_1 - \mu_2)$ . Equation 2.53 (with  $\alpha = 0$ ) can be expanded in a bivariate Taylor's series about the point  $(\frac{1}{2}(\mu_1 - \mu_2), 0)$ . Taking the difference of these expansions gives

$$\begin{aligned}
(2.54) \quad P_2 - P_D &\doteq (\zeta - \eta) \Phi_{10} - \tau \Phi_{01} + \frac{1}{2} [(\zeta^2 - \eta^2) \Phi_{20} - 2\eta\tau \Phi_{11} - \tau^2 \Phi_{02}] \\
&+ \frac{1}{6} [(\zeta^3 - \eta^3) \Phi_{30} - 3\eta^2 \tau \Phi_{21} - 3\eta\tau^2 \Phi_{12} - \tau^3 \Phi_{03}] \\
&+ \frac{1}{24} [(\zeta^4 - \eta^4) \Phi_{40} - 4\eta^3 \tau \Phi_{31} - 6\eta^2 \tau^2 \Phi_{22} - 4\eta\tau^3 \Phi_{13} - \tau^4 \Phi_{04}]
\end{aligned}$$

$$\text{where } \Phi_{k\ell} = \frac{\partial^{k\ell} \Phi(tu^{-1/2})}{\partial t^k \partial u^\ell} \quad \left| \begin{array}{l} t = \frac{1}{2}(\mu_1 - \mu_2) \\ u = 1 \end{array} \right. \quad \text{for } k, \ell = 0, 1, 2, 3, 4.$$

Squaring equation 2.54 and retaining all relevant terms results in

$$\begin{aligned}
(2.55) \quad (P_2 - P_D)^2 &\doteq (\zeta - \eta)^2 \Phi_{10}^2 - 2\tau(\zeta - \eta) \Phi_{10} \Phi_{01} + \tau^2 \Phi_{01}^2 \\
&+ \frac{1}{4} [(\zeta^2 - \eta^2)^2 \Phi_{20}^2 + 4\eta^2 \tau^2 \Phi_{11}^2 + \tau^4 \Phi_{02}^2 \\
&- 4\tau\eta(\zeta^2 - \eta^2) \Phi_{20} \Phi_{11} - 2\tau^2(\zeta^2 - \eta^2) \Phi_{20} \Phi_{02} + 4\tau^3 \eta \Phi_{11} \Phi_{02}] \\
&+ (\zeta - \eta)(\zeta^2 - \eta^2) \Phi_{10} \Phi_{20} - \tau(\zeta^2 - \eta^2) \Phi_{01} \Phi_{20} - 2\tau\eta(\zeta - \eta) \Phi_{10} \Phi_{11} \\
&+ 2\tau^2 \eta \Phi_{01} \Phi_{11} - \tau^2(\zeta - \eta) \Phi_{10} \Phi_{02} + \tau^3 \Phi_{01} \Phi_{02} \\
&+ \frac{1}{3} [(\zeta - \eta)(\zeta^3 - \eta^3) \Phi_{10} \Phi_{30} - \tau(\zeta^3 - \eta^3) \Phi_{01} \Phi_{30} - 3\tau\eta^2(\zeta - \eta) \Phi_{10} \Phi_{21} \\
&+ 3\tau^2 \eta^2 \Phi_{01} \Phi_{21} - 3\tau^2 \eta(\zeta - \eta) \Phi_{10} \Phi_{12} + 3\tau^3 \eta \Phi_{01} \Phi_{12} \\
&- \tau^3(\zeta - \eta) \Phi_{10} \Phi_{03} + \tau^4 \Phi_{01} \Phi_{03}].
\end{aligned}$$

Taking the expectation of equation 2.55 with respect to  $\zeta$ ,  $\eta$  and  $\tau$  gives

$$\begin{aligned}
(2.56) \quad E[(P_2 - P_D)^2] &= n_2^{-1} \Phi_{10}^2 + 2(n_1 + n_2 - 2)^{-1} \Phi_{01}^2 \\
&+ \frac{1}{4} (n_1^{-1} n_2^{-1} + n_2^{-2}) \Phi_{10} \Phi_{30} + \frac{1}{4} n_1^{-1} n_2^{-1} \Phi_{20}^2 \\
&+ \frac{1}{2} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) (\Phi_{01} \Phi_{21} + \Phi_{11}^2) \\
&+ (n_1 + n_2 - 2)^{-1} n_2^{-1} \Phi_{10} \Phi_{12} + 10(n_1 + n_2 - 2)^{-2} \Phi_{01} \Phi_{02} + O_3.
\end{aligned}$$

For the estimators  $P_{DS}^{**}$ ,  $P_G$  and  $P_S$ , the specific versions of equations 2.53 are more complicated than is the version for  $P_D$ ; and subsequent computations are considerably more extensive. Except for the addition of a binomial expansion of  $(1 + \alpha)^{-1/2}$ , the methods used in obtaining the mean square errors of these three estimators are essentially the same as those demonstrated for  $P_D$ . Therefore, only the mean square errors for  $P_{DS}^{**}$ ,  $P_G$  and  $P_S$  are given below.

$$\begin{aligned}
(2.57) \quad E[(P_2 - P_{DS}^{**})^2] &= n_2^{-1} \Phi_{10}^2 + 2(n_1 + n_2 - 2)^{-1} \Phi_{01}^2 \\
&+ \frac{1}{4} (n_1^{-1} n_2^{-1} + n_2^{-2}) \Phi_{10} \Phi_{30} + \frac{1}{4} n_1^{-1} n_2^{-1} \Phi_{20}^2 \\
&+ \frac{1}{2} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) (\Phi_{01} \Phi_{21} + \Phi_{11}^2) \\
&+ (n_1 + n_2 - 2)^{-1} n_2^{-1} \Phi_{10} \Phi_{12} + 10(n_1 + n_2 - 2)^{-2} \Phi_{01} \Phi_{02} \\
&- [(n_1 + n_2 - 4)^{-1} n_2^{-1} - \frac{1}{4} (n_1 + n_2 - 4)^{-2} (\mu_1 - \mu_2)^2] \Phi_{10}^2 \\
&- \frac{1}{2} (n_1 + n_2 - 4)^{-1} n_2^{-1} (\mu_1 - \mu_2) \Phi_{10} \Phi_{20} \\
&- (n_1 + n_2 - 4)^{-1} (n_1 + n_2 - 2)^{-1} (\Phi_{01} \Phi_{11} + \Phi_{10} \Phi_{02}) + O_3.
\end{aligned}$$

$$\begin{aligned}
(2.58) \quad E[(P_2 - P_G)^2] &= n_2^{-1} \Phi_{10}^2 + 2(n_1 + n_2 - 2)^{-1} \Phi_{01}^2 \\
&+ \frac{1}{4} (n_1^{-1} n_2^{-1} + n_2^{-2}) \Phi_{10} \Phi_{30} + \frac{1}{4} n_1^{-1} n_2^{-1} \Phi_{20}^2 \\
&+ \frac{1}{2} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) (\Phi_{01} \Phi_{21} + \Phi_{11}^2) \\
&+ (n_1 + n_2 - 2)^{-1} n_2^{-1} \Phi_{10} \Phi_{12} + 10(n_1 + n_2 - 2)^{-2} \Phi_{01} \Phi_{02} \\
&- \left[ \frac{1}{2} - \frac{1}{16} (\mu_1 - \mu_2)^2 \right] n_2^{-2} \Phi_{10}^2 - \frac{1}{4} (\mu_1 - \mu_2) n_2^{-2} \Phi_{10} \Phi_{20} \\
&- \frac{1}{2} (\mu_1 - \mu_2) (n_1 + n_2 - 2)^{-1} n_2^{-1} (\Phi_{01} \Phi_{11} + \Phi_{10} \Phi_{02}) + O_3.
\end{aligned}$$

$$\begin{aligned}
(2.59) \quad E[(P_2 - P_S)^2] &= n_2^{-1} \Phi_{10}^2 + 2(n_1 + n_2 - 2)^{-1} \Phi_{01}^2 \\
&+ \frac{1}{4} (n_1^{-1} n_2^{-1} + n_2^{-2}) \Phi_{10} \Phi_{30} + \frac{1}{4} n_1^{-1} n_2^{-1} \Phi_{20}^2 \\
&+ \frac{1}{2} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) (\Phi_{01} \Phi_{21} + \Phi_{11}^2) \\
&+ (n_1 + n_2 - 2)^{-1} n_2^{-1} \Phi_{10} \Phi_{12} + 10(n_1 + n_2 - 2)^{-2} \Phi_{01} \Phi_{02} \\
&- \left[ \frac{1}{4} - \frac{1}{64} (\mu_1 - \mu_2)^2 \right] n_2^{-2} \Phi_{10}^2 - \frac{1}{8} (\mu_1 - \mu_2) n_2^{-2} \Phi_{10} \Phi_{20} \\
&- \frac{1}{4} (\mu_1 - \mu_2) (n_1 + n_2 - 2)^{-1} n_2^{-1} (\Phi_{01} \Phi_{11} + \Phi_{10} \Phi_{02}) + O_3.
\end{aligned}$$

Next consider the estimators  $P_O^*$  and  $P_{OS}^*$  which are based on Okamoto's (1963) expansion for  $P_2$ . Note that both estimators can be written in the general form



$$(2.60) \quad \hat{P}_2^* = \Phi_{00} \left( \left[ \frac{1}{2}(\mu_1 - \mu_2) + \eta \right] / [1 + \tau]^{1/2} [1 + \alpha]^{1/2} \right) \\ + \frac{1}{8} (n_1^{-1} + n_2^{-1}) \Phi_{20} \left( \left[ \frac{1}{2}(\mu_1 - \mu_2) + \eta \right] / [1 + \tau]^{1/2} [1 + \alpha]^{1/2} \right)$$

where  $\alpha$  takes on the values 0 and  $2(n_1 + n_2 - 4)^{-1}$  for  $P_O^*$  and  $P_{OS}^*$ , respectively.

As for the case when  $\sigma^2$  is known,  $(1 + \alpha)^{-1/2}$  can be expanded in a binomial series and the estimators as given in equation 2.60 can be expanded in a bivariate Taylor's series about the point  $(\frac{1}{2}(\mu_1 - \mu_2), 0)$ .

Taking the difference of the resulting expression for  $\hat{P}^*$  and the expansion of  $P_2$  (defined by equation 2.52) gives

$$(2.61) \quad P_2 - \hat{P}_2^* = (\zeta - \eta) \Phi_{10} - \tau \Phi_{01} \\ + \frac{1}{2} \left[ \zeta^2 - (\eta - [\frac{1}{2}(\mu_1 - \mu_2) + \eta]) \left( \frac{\alpha}{2} - \frac{3\alpha^2}{8} \right) \right]^2 - \frac{1}{4} (n_1^{-1} + n_2^{-1}) \Phi_{20} \\ - \tau \left[ \eta - (\frac{1}{2}[\mu_1 - \mu_2] + \eta) \left( \frac{\alpha}{2} - \frac{3\alpha^2}{8} \right) \right] \Phi_{11} - \frac{1}{2} \tau^2 \Phi_{02} \\ + \frac{1}{6} \left[ \zeta^3 - (\eta - [\frac{1}{2}(\mu_1 - \mu_2) + \eta]) \left( \frac{\alpha}{2} - \frac{3\alpha^2}{8} \right) \right]^3 - \\ - \frac{3}{4} \left( \eta - [\frac{1}{2}(\mu_1 - \mu_2) + \eta] \left( \frac{\alpha}{2} - \frac{3\alpha^2}{8} \right) \right) (n_1^{-1} + n_2^{-1}) \Phi_{30} \\ - \frac{1}{2} \tau^2 \left[ \eta - (\frac{1}{2}[\mu_1 - \mu_2] + \eta) \left( \frac{\alpha}{2} - \frac{3\alpha^2}{8} \right) \right] \Phi_{12} \\ - \frac{1}{2} \tau \left[ (\eta - [\frac{1}{2}(\mu_1 - \mu_2) + \eta]) \left( \frac{\alpha}{2} - \frac{3\alpha^2}{8} \right) \right]^2 + \frac{1}{4} (n_1^{-1} + n_2^{-1}) \Phi_{21} \\ - \frac{1}{6} \tau^3 \Phi_{03}.$$

Squaring equation 2.61 and taking the expectation with respect to  $\zeta$ ,  $\eta$  and  $\tau$  lead to

$$\begin{aligned}
(2.62) \quad E[(P_2 - P_0^*)^2] &= n_2^{-1} \Phi_{10}^2 + \left( \frac{n_1^{-2} + n_2^{-2}}{64} + \frac{9n_1^{-1} n_2^{-1}}{32} \right) \Phi_{20}^2 \\
&\quad + \frac{3n_1^{-1} n_2^{-1} + 3n_2^{-2}}{8} \Phi_{10} \Phi_{30} \\
&\quad + 2(n_1 + n_2 - 2)^{-1} \Phi_{01}^2 + \frac{1}{2} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) \Phi_{11}^2 \\
&\quad + (n_1 + n_2 - 2)^{-1} n_2^{-1} \Phi_{10} \Phi_{12} + \frac{3}{4} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) \Phi_{01} \Phi_{21} \\
&\quad + 10(n_1 + n_2 - 2)^{-2} \Phi_{01} \Phi_{02} + \frac{1}{4} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) \Phi_{20} \Phi_{02} + O_3,
\end{aligned}$$

and

$$\begin{aligned}
(2.63) \quad E[(P_2 - P_{OS}^*)^2] &= [n_2^{-1} + 2(n_1 + n_2 - 4)^{-1} n_2^{-1} + (n_1 + n_2 - 4)^{-2} (\mu_1 - \mu_2)^2] \Phi_{10}^2 \\
&\quad + \left( \frac{n_1^{-2} + n_2^{-2}}{64} + \frac{9n_1^{-1} n_2^{-1}}{32} \right) \Phi_{20}^2 + \frac{3n_1^{-1} n_2^{-1} + 3n_2^{-2}}{8} \Phi_{10} \Phi_{30} \\
&\quad + 2(n_1 + n_2 - 2)^{-1} \Phi_{01}^2 + \frac{1}{2} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) \Phi_{11}^2 \\
&\quad + (n_1 + n_2 - 2)^{-1} n_2^{-1} \Phi_{10} \Phi_{12} + \frac{1}{4} (n_1 + n_2 - 4)^{-1} (n_1^{-1} - 3n_2^{-1}) (\mu_1 - \mu_2) \Phi_{10} \Phi_{20} \\
&\quad + 2(n_1 + n_2 - 4)^{-1} (n_1 + n_2 - 2)^{-1} (\mu_1 - \mu_2) \Phi_{10} \Phi_{02} \\
&\quad + 4(n_1 + n_2 - 4)^{-1} (n_1 + n_2 - 2)^{-1} (\mu_1 - \mu_2) \Phi_{11} \Phi_{01} \\
&\quad + \frac{3}{4} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) \Phi_{01} \Phi_{21} \\
&\quad + 10(n_1 + n_2 - 2)^{-2} \Phi_{01} \Phi_{02} + \frac{1}{4} (n_1 + n_2 - 2)^{-1} (n_1^{-1} + n_2^{-1}) \Phi_{20} \Phi_{02} + O_3.
\end{aligned}$$

## DISCUSSION

Comparison of the mean square errors for the various estimators leads to some interesting results. If the two estimators not motivated by the assumption that  $\pi_1$  and  $\pi_2$  are normal populations (that is,  $P_R$  and  $P_U$ ) are compared, it can be seen that for large values of  $|\mu_1 - \mu_2|$ ,  $P_R$  is a "better" (in the sense of mean square error) estimator of  $P_2$  than is  $P_U$ . Making use of the normality of  $\pi_1$  and  $\pi_2$ , as might be expected, is advantageous. Support of the conclusion that any of  $P_D, P_G, P_S, P_{DS}^{**}, P_O^*, P_{OS}^*$  is a better estimator than either  $P_R$  or  $P_U$  is given below. Choosing among the six estimators relying on the normality of  $\pi_1$  and  $\pi_2$  is not trivial. However,  $P_D$  seems in general to be less satisfactory than the alternatives.

Consider first the estimators  $P_R$  and  $P_U$  and their mean square errors given by equations 2.37 and 2.38, respectively. Note that the terms with coefficients  $n_2^{-1}$  and  $n_1^{-1} n_2^{-1}$  are the same in both equations. The remaining term with the coefficient of  $n_2^{-2}$  for  $P_R$  is  $\frac{3}{8}(\Phi_2^{(2)} - \Phi_2) + \frac{1}{4}\Phi_2^{(2)}$ . For large values of  $|\mu_1 - \mu_2|$  this expression is seen to be negative. However, the remaining term (with the coefficient  $n_2^{-2}$ ) of  $P_U$  is  $\frac{1}{8}(\Phi_2 - \Phi_2^{(2)}) + \frac{1}{4}\Phi_1^2$ , which expression is always positive. (For definitions of  $\Phi_{kl}^{(r)}$  and  $\Phi_k^{(r)}$ , see the appendix.) Thus for large values of  $|\mu_1 - \mu_2|$ ,  $P_R$  is concluded to be a better estimator of  $P_2$

than is  $P_U$ , despite the intuitive appeal of  $P_U$ .

Since the estimators  $P_D, P_G, P_S, P_{DS}^{**}, P_O^*, P_{OS}^*$  make use of additional information about  $\pi_1$  and  $\pi_2$ , it might be expected that the mean square error of any of these estimators could be shown to be smaller than that of either  $P_R$  or  $P_U$ . It is perhaps surprising that as quantitatively crude an argument as the following one is sufficient to support this conclusion.

The mean square errors of  $P_R$  and  $P_U$  are the same whether or not  $\sigma^2$  is known, while the mean square errors of  $P_D$  and the other estimators motivated by the normality of  $\pi_1$  and  $\pi_2$  are larger when  $\sigma^2$  is unknown than when  $\sigma^2$  is known. Thus it suffices here to treat the case when  $\sigma^2$  is unknown. Consider the first order terms of the mean square errors of  $P_R$  (or  $P_U$ , since such terms are the same for these two estimators) as given by equation 2.37 (or equation 2.38) and of  $P_D$  (or  $P_G, P_S, P_{DS}^{**}, P_O^*,$  or  $P_{OS}^*$ ) as given by equation 2.56 (or any of equations 2.57, 2.58, 2.59, 2.62, 2.63). Define by  $G_1$  their difference; thus

$$(2.64) \quad G_1 = E[(P_2 - P_R)^2] - E[(P_2 - P_D)^2]$$

to  $O_2$ . Rewriting  $G_1$  using equations 2.37 and 2.56, and making use of definitions in the appendix give

$$(2.65) \quad G_1(y) = n_2^{-1} \Phi_0(y)[1 - \Phi_0(y)] - \frac{1}{4}[n_2^{-1} + 2(n_1 + n_2 - 2)^{-1}]y^2 \Phi_1(y)$$

for  $y < 0$ ,

where  $y = \frac{1}{2}(\mu_1 - \mu_2)$ . By finding the minimum value of  $G_1$  (over the range of  $y$ ) and showing this minimum value to be positive, it will have been

demonstrated that  $P_D$  is the better (to  $O_2$ ) estimator of  $P_2$  for all values of  $D^2$ . Hence consider next  $G_1'(y)$ ,

$$(2.66) \quad G_1'(y) = (n_2^{-1} - 2n_2^{-1}\Phi_0(y) + \frac{1}{2}[n_2^{-1} + 2(n_1+n_2-2)^{-1}][y^3-y]\Phi_1(y))\Phi_1(y).$$

Since  $\Phi_0(y) \leq \frac{1}{2}$ , it follows immediately that for  $y \geq -1$ ,  $G_1'(y)$  is non-negative. When  $y < -1$ , the behavior of  $G_1'(y)$  is not so apparent.

However, whenever  $G_1'(y) = 0$ ,

$$(2.67) \quad G_2(y) = 1 - 2\Phi_0(y) + \frac{1}{2}[1 + 2n_2(n_1+n_2-2)^{-1}](y^3-y)\Phi_1(y) = 0.$$

It will now be shown that  $G_2(y)$  does not take on the value zero for  $y < -1$ . In fact,  $G_2(y)$  has only one local minimum for  $y < -1$ , and that minimal value of  $G_2(y)$  is positive. To find this minimum of  $G_2(y)$ , consider  $G_2'(y)$ , which can be shown to be

$$(2.68) \quad G_2'(y) = [\frac{1}{2} - 3y^2 + \frac{1}{2}y^4][1 + 2n_2(n_1+n_2-2)^{-1}]\Phi_1(y).$$

Setting equation 2.68 equal to zero and solving for  $y$  gives only one relevant solution,  $y_0$ ,

$$(2.69) \quad y_0 = -2.412.$$

A check of  $G_2''(y)$  shows that  $y_0$  does indeed yield a minimum for  $G_2'(y)$ . Substitution of  $y_0$  into equation 2.67 gives

$$(2.70) \quad G_2(y_0) = .1272[1 + 2n_2(n_1 + n_2 - 2)^{-1}].$$

It follows that  $G_1'(y)$  is nonnegative for all  $y < 0$ . Thus it is concluded that  $G_1(y)$  attains its maximum and its minimum values at  $y = 0$  and in the limit as  $y \rightarrow -\infty$ . From equation 2.65, the maximum and minimum values of  $G_1(y)$  are given by

$$(2.71) \quad G_1(0) = \frac{1}{4}n_2^{-1}, \text{ and}$$

$$(2.72) \quad \lim_{y \rightarrow -\infty} G_1(y) = 0.$$

Thus it has been proved that (to  $O_2$ ) the mean square error for  $P_R$  (or for  $P_0$ ) exceeds that for  $P_U$  (or for  $P_G, P_S, P_{DS}^{**}, P_O^*$  or  $P_{OS}^*$ ) regardless of the value of  $D^2$ .

### PART III. OPTIMALITY OF PRINCIPAL COMPONENTS

# CASE WHEN VECTOR VARIABLES ARE REAL-VALUED

The principal components of a  $p \times 1$  vector-valued random variable,  $x$ , (from any distribution for which expectation and variance are meaningful) can be characterized as linear combinations of  $x_1, x_2, \dots, x_p$  with particular variance properties. Hotelling (1933) first introduced principal components; Rao (1964), Darroch (1965) and Okamoto and Kanazawa (1968) have characterized them in terms of various optimal properties.

The study of principal components is relevant when it is desirable to make assertions or inferences about a  $p \times 1$  vector-valued random variable in terms of fewer than  $p$  characteristics (or linear combinations of  $x_1, x_2, \dots, x_p$ ). For example, often it is the linear combination of  $x_1, x_2, \dots, x_p$  with the largest variance that is sought in order to investigate individual variation using the "best" single indicator. The logical extension of this example would involve the "best  $k$ " ( $k < p$ ) indicators. It is in the definition of "best" that the characterizations of principal components by Rao (1964), Darroch (1965) and Okamoto and Kanazawa (1968) differ.

Let  $x = (x_1, x_2, \dots, x_p)'$  be a real-valued random vector with mean,  $E(x) = (0, 0, \dots, 0)'$ , and real covariance matrix,  $E(xx') = \Sigma$ . Also, let  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$  be the eigenvalues of  $\Sigma$  in order of decreasing magnitude; and let  $\gamma_1, \gamma_2, \dots, \gamma_p$  be the corresponding orthonormal



eigenvectors. Then  $\gamma_1'x, \gamma_2'x, \dots, \gamma_p'x$  are the principal components of  $x$ . Denote  $\gamma_i'x$  by  $\xi_i$  ( $i = 1, 2, \dots, p$ ).

In terms of geometry, the set of principal components effectively rotates the coordinate axes to a new (mutually-orthogonal) system of coordinates with useful statistical properties. For example, the first principal component is that (normalized) linear combination with maximum variance. Thus the largest variance component of  $x$  lies along the first axis in the new coordinate system. The second principal component is that (normalized) linear combination (orthogonal to the first principal component) with maximum variance; hence the second largest variance component (independent of the largest variance component) of  $x$  lies along the second axis in the new coordinate system; and so on.

The characterization of the first  $k$  ( $k \leq p$ ) principal components given by Rao (1964) is that linear form,  $y = T'x$  with a real  $p \times k$  matrix  $T$ , which minimizes the Euclidean norm of the residual matrix of  $x$  after subtraction of its best linear predictor based on  $y$ . In other words, Rao considered the problem

$$(3.1) \quad \text{Minimize } \|E[(x - AT'x)(x - AT'x)']\|$$

subject to the conditions that  $A$  is a  $p \times k$  real matrix  
and  $T$  is a  $p \times k$  real matrix,

where  $\| \quad \|$  denotes the Euclidean norm; and he obtained the solution

$$AT'x = \sum_{i=1}^k \gamma_i \xi_i.$$

The problem Darroch (1965) considered is

- (3.2) Minimize  $\text{tr}(E[(x - Ay)(x - Ay)'])$   
 subject to the conditions that  $A$  is a  $p \times k$  real matrix  
 and  $y$  is a random  $k$ -vector with  $E(y) = 0$ ;

and he obtained the solution  $Ay = \sum_{i=1}^k \gamma_i \xi_i$ .

Okamoto and Kanazawa (1968) treated the general case (of which problems 3.1 and 3.2 are special cases),

- (3.3) Minimize simultaneously the eigenvalues of  $E[(x - Ay)(x - Ay)']$   
 subject to the conditions that  $A$  is a  $p \times k$  real matrix  
 and  $y$  is a random  $k$ -vector with  $E(y) = 0$ ;

and obtained the solution  $Ay = \sum_{i=1}^k \gamma_i \xi_i$ .

# CASE WHEN VECTOR VARIABLES ARE COMPLEX-VALUED

The results for the case of complex variables presented in this section are strictly analogous to the results for the case of real variables. Since the result obtained by Okamoto and Kanazawa (1968) for the case of real variables is a general result encompassing those obtained by Rao (1964) and Darroch (1965), only the analogous general result for complex variables is presented here. For the sake of completeness, aspects of the proof of this more general optimality property which are unaffected by the complex character of the variables are included although the argument is as Okamoto and Kanazawa have presented it.

Let  $\mathbf{x} = (x_1, x_2, \dots, x_p)'$  be a complex-valued random vector with mean,  $E(\mathbf{x}) = (0, 0, \dots, 0)'$ , and covariance matrix  $E(\mathbf{x}\mathbf{x}^*) = \Sigma$ , where  $\mathbf{x}^*$  denotes the transpose of the complex conjugate of  $\mathbf{x}$ .

Note that  $\Sigma$  is a  $p \times p$  Hermitian matrix. Let

$\lambda_1(\Sigma) \geq \lambda_2(\Sigma) \geq \dots \geq \lambda_p(\Sigma) \geq 0$  be the eigenvalues of  $\Sigma$  in order of

decreasing magnitude. (Since  $\Sigma$  is Hermitian,  $\lambda_i$  is real for  $i = 1, 2, \dots, p$ .) Let  $\gamma_1(\Sigma), \gamma_2(\Sigma), \dots, \gamma_p(\Sigma)$  be the corresponding orthonormal eigenvectors; and let the principal components of  $x$ ,  $\gamma_1(\Sigma)^* x, \gamma_2(\Sigma)^* x, \dots, \gamma_p(\Sigma)^* x$ , be denoted by  $\xi_1, \xi_2, \dots, \xi_p$ .

Let  $\mathcal{A} = \mathcal{A}_p$  be the set of all Hermitian matrices of order  $p$ . A partial order in the set  $\mathcal{A}$  is defined as usual:  $A \geq B$  if and only if  $A - B \in \mathcal{A}$ . For any  $A \in \mathcal{A}$  let  $\lambda_1(A) \geq \lambda_2(A) \geq \dots \geq \lambda_p(A) \geq 0$  be the eigenvalues of  $A$  in order of decreasing magnitude. The following lemma is stated without proof.

Lemma 1. A necessary and sufficient condition for a real-valued function  $f(A)$  defined on  $\mathcal{A}$  to be

(i) strictly increasing, that is,  $f(A) \geq f(B)$  if

$A \geq B$ , and  $f(A) > f(B)$  if moreover  $A \neq B$ ,

and

(ii) invariant under unitary transformation, that is,

$f(P^* A P) = f(A)$  for any unitary matrix  $P$ ,

is that  $f(A)$  is identical to some function  $g(\lambda_1(A), \lambda_2(A), \dots, \lambda_p(A))$  of

the eigenvalues of  $A$  which is strictly increasing in each argument.

Note that the trace and the Euclidean norm are both such functions  $f$ .

Lemma 2. Let  $\gamma_1, \gamma_2, \dots, \gamma_k$  be any set of first  $k$  eigenvectors of a  $p \times p$  Hermitian matrix,  $A$ . Then

$$\lambda_{k+1}(A) = \sup_{\substack{\gamma_j^* x = 0 \\ j=1, 2, \dots, k}} \frac{x^* Ax}{x^* x}$$

Proof. Define  $A_1$  and  $A_2$ , real  $p \times p$  matrices, by  $A = A_1 + iA_2$ ; and denote by  $C$  the  $2p \times 2p$  real matrix  $\begin{pmatrix} A_1 & -A_2 \\ A_2 & A_1 \end{pmatrix}$ . Note that  $C$  is symmetric since  $A$  is Hermitian; and that  $\lambda_{2j}(C) = \lambda_j(A)$  (see Bellman (1960, p. 84)). Let  $v_j$  denote a  $j^{\text{th}}$  eigenvector for  $C$  ( $j \leq 2k$ ); and let  $v_j^{(1)}$  and  $v_j^{(2)}$ , real  $k$ -vectors, be defined by  $v_j = \begin{pmatrix} v_j^{(1)} \\ v_j^{(2)} \end{pmatrix}$ . It is asserted that there is a 1:1 relationship between  $v_{2j}$  and  $\gamma_j$  for  $j = 1, 2, \dots, k$ .

(i) Let  $v_{2j}$  be any  $2j^{\text{th}}$  eigenvector for  $C$  ( $j \leq k$ ). Then

$$Cv_{2j} = \begin{pmatrix} A_1 v_{2j}^{(1)} - A_2 v_{2j}^{(2)} \\ A_2 v_{2j}^{(1)} + A_1 v_{2j}^{(2)} \end{pmatrix} = \lambda_{2j}(C) \begin{pmatrix} v_{2j}^{(1)} \\ v_{2j}^{(2)} \end{pmatrix}, \text{ which implies}$$

$$(A_2 v_{2j}^{(1)} + A_1 v_{2j}^{(2)}) = \lambda_{2j}(C) v_{2j}^{(2)}. \text{ Define } \gamma_j \text{ by } \gamma_j = v_{2j}^{(2)} + i v_{2j}^{(1)}. \text{ Then}$$

$\gamma_j$  is a  $j^{\text{th}}$  eigenvector of  $A$  since

$$\begin{aligned}
A\gamma_j &= (A_1 + iA_2)(v_{2j}^{(1)} + iv_{2j}^{(2)}) = A_1 v_{2j}^{(1)} - A_2 v_{2j}^{(2)} + iA_2 v_{2j}^{(1)} + iA_1 v_{2j}^{(2)} \\
&= \lambda_{2j}(C)v_{2j}^{(1)} + i\lambda_{2j}(C)v_{2j}^{(2)} = \lambda_{2j}(C)(v_{2j}^{(1)} + iv_{2j}^{(2)}) = \lambda_{2j}(C)\gamma_j \\
&= \lambda_j \gamma_j \quad \text{since } \lambda_{2j}(C) = \lambda_j(A).
\end{aligned}$$

Thus  $Cv_{2j} = \lambda_j \gamma_j$ .

(ii) Let  $\gamma_j$  be any  $j^{\text{th}}$  eigenvector for  $A$  ( $j \leq k$ ). Define  $\gamma_j^{(1)}$  and  $\gamma_j^{(2)}$  by  $\gamma_j = \gamma_j^{(1)} + i\gamma_j^{(2)}$ ; then  $(A_1 + iA_2)\gamma_j = (A_1 + iA_2)(\gamma_j^{(1)} + i\gamma_j^{(2)})$ .

Define  $v_{2j}$  by  $\begin{pmatrix} \gamma_j^{(1)} \\ \gamma_j^{(2)} \end{pmatrix}$ . Then  $v_{2j}$  is a  $2j^{\text{th}}$  eigenvector for  $C$  since

$$\begin{aligned}
Cv_{2j} &= \begin{pmatrix} A_1 & -A_2 \\ A_2 & A_1 \end{pmatrix} \begin{pmatrix} \gamma_j^{(1)} \\ \gamma_j^{(2)} \end{pmatrix} = \begin{pmatrix} A_1 \gamma_j^{(1)} - A_2 \gamma_j^{(2)} \\ A_2 \gamma_j^{(1)} + A_1 \gamma_j^{(2)} \end{pmatrix} = \lambda_j(A) \begin{pmatrix} \gamma_j^{(1)} \\ \gamma_j^{(2)} \end{pmatrix} = \\
&= \lambda_{2j}(C)v_{2j}.
\end{aligned}$$

Note that analogous reasoning relates  $v_{2j-1}$  and  $\gamma_j$ .

Next consider the assertion  $\sup_{\mathbb{R}_k} \frac{(v, Cv)}{(v, v)} = \sup_{\mathbb{K}_k} \frac{(\gamma, A\gamma)}{(\gamma, \gamma)}$  where  $\mathbb{R}_k$

and  $\mathbb{K}_k$  are the (real and complex, respectively) regions determined by the orthogonality relations  $(v, v^{2i}) = 0$ ,  $(\gamma, \gamma^i) = 0$  for  $i = 1, 2, \dots, k-1$ , and  $v \neq 0$ ,  $\gamma \neq 0$ . Let

$\begin{pmatrix} \gamma_j^{(1)} \\ \gamma_j^{(2)} \end{pmatrix}$  for  $j = 1, 2, \dots, p$  be a set of  $p$  eigenvectors for  $C$ . Then

$(\gamma_j^{(1)} + i\gamma_j^{(2)})$  for  $j = 1, 2, \dots, p$  is a set of  $p$  eigenvectors for  $A$ . Consider an arbitrary vector  $\gamma$  satisfying the orthogonality relations given above. Then  $\gamma$  can be written  $\gamma = \sum_{j=1}^p (u_j^{(1)} + iu_j^{(2)})(\gamma_j^{(1)} + i\gamma_j^{(2)})$  for some real  $p$ -vectors  $u_j^{(1)}$  and  $u_j^{(2)}$ ,  $j = 1, 2, \dots, p$ . It follows that

$$(\gamma, A\gamma) = (\gamma^* A\gamma) = \sum_{j=1}^p \lambda_j(A)(u_j^{(1)} - iu_j^{(2)})(u_j^{(1)} + iu_j^{(2)}) = \sum_{j=1}^p \lambda_j(A)[(u_j^{(1)})^2 + (u_j^{(2)})^2],$$

and  $(\gamma, \gamma) = (\gamma^* \gamma) = \sum_{j=1}^p (u_j^{(1)} - iu_j^{(2)})(u_j^{(1)} + iu_j^{(2)}) = \sum_{j=1}^p [(u_j^{(1)})^2 + (u_j^{(2)})^2]$ . Define

$$v = \begin{pmatrix} \sum_{j=1}^p u_j^{(1)} \gamma_j^{(1)} + \sum_{j=1}^p u_j^{(2)} (-\gamma_j^{(2)}) \\ \sum_{j=1}^p u_j^{(1)} \gamma_j^{(2)} + \sum_{j=1}^p u_j^{(2)} \gamma_j^{(1)} \end{pmatrix} = \sum_{i=1}^{2p} s_i \gamma_j^i \text{ where } \begin{aligned} s_i &= u_j^{(1)} \text{ for } k=1, 2, \dots, p \\ &= u_j^{(2)} \text{ for } \\ &k = p+1, \dots, 2p. \end{aligned}$$

Then  $(v, Cv) = \sum_{i=1}^{2p} \lambda_i(C) x_i^2 = 2 \sum_{i=1}^p \lambda_i(C)[(u_i^{(1)})^2 + (u_i^{(2)})^2]$ , and

$$(v, v) = \sum_{i=1}^{2p} s_i^2 = 2 \sum_{i=1}^p [(u_i^{(1)})^2 + (u_i^{(2)})^2].$$

As  $\gamma$  spans out the vector space of  $A$ , corresponding  $v$  spans out the vector space of  $C$ . Thus  $\frac{(v, Cv)}{(v, v)} = \frac{(\gamma, A\gamma)}{(\gamma, \gamma)}$  as  $v, \gamma$  simultaneously

span out the vector spaces of  $C$  and  $A$ ; and hence  $\sup \frac{(v, Cv)}{(v, v)} =$

$\sup \frac{(\gamma, A\gamma)}{(\gamma, \gamma)}$  and the suprema (if achieved) occur simultaneously (or are analogous limit points).

From previous work  $\lambda_{k+1}(A) = \lambda_{2k+2}(C) = \sup_{R_k} \frac{(v, Cv)}{(v, v)} = \sup_{K_k} \frac{(\gamma, A\gamma)}{(\gamma, \gamma)}$ .

By the same argument, the supremum is attained if and only if  $\gamma$  is an eigenvector of  $A$  associated with  $\lambda_k(A)$ .

Dually, if  $\gamma_p, \gamma_{p-1}, \dots, \gamma_{p-k+1}$  is any set of last  $k$  eigenvectors of  $A$ , it follows that  $\lambda_{p-k}(A) = \inf_{\substack{\gamma_i^* \gamma = 0 \\ i=p, \dots, p-k+1}} \frac{\gamma^* A \gamma}{\gamma^* \gamma}$ . The infimum is attained if and only if  $\gamma$  is an eigenvector of  $A$  associated with  $\lambda_{p-k}(A)$ .

Let  $M_k(A)$  for  $k = 1, 2, \dots, p$  denote the linear subspace spanned by the eigenvectors corresponding to the eigenvalues larger than  $\lambda_k(A)$ . Note that  $M_k(A)$  does not necessarily involve all of the eigenvectors corresponding to  $\lambda_1(A), \lambda_2(A), \dots, \lambda_{k-1}(A)$  since it is possible that  $\lambda_{k-1}(A) = \lambda_k(A)$ . For any matrix  $L$ , denote by  $M(L)$  the linear subspace spanned by the column vectors of  $L$ .

Lemma 3. For any  $p \times p$  Hermitian matrix  $A$ , it holds that

$$\lambda_{k+1}(A) = \inf_L \sup_{L^* \gamma = 0} \frac{\gamma^* A \gamma}{\gamma^* \gamma}$$

where the infimum is taken over all complex matrices  $L$  with  $p$  rows and with rank less than or equal to  $k$ , and where the supremum is taken over  $p$ -vectors such that  $L^* \gamma = 0$ . The infimum is attained if (but not only if)  $M(L)$  contains any first  $k$  eigenvectors of  $A$ .

Proof. The method of proof is as in the proof of Lemma 2. Since the



result for real matrices is well-known as the Courant-Fischer min-max theorem, it suffices here to show the 1:1 relationship of  $C$  and  $A$  and to demonstrate an analogous relationship between the matrices  $J$  and  $L$ , where

$$\lambda_{2k+2}(C) = \inf_J \sup_{J'v=0} \frac{v'Cv}{v'v}.$$

It follows almost immediately from the proof of Lemma 2 that  $J = \begin{pmatrix} J_1 & -J_2 \\ J_2 & J_1 \end{pmatrix}$  and  $L = J_1 + iJ_2$ .

Lemma 4. For any  $A \in \mathcal{A}$ , any positive integer  $k$  and any matrix  $L$  with  $p$  rows and with rank less than  $k$ , it holds that

$$\sup_{L^* \gamma = 0} \frac{\gamma^* A \gamma}{\gamma^* \gamma} \geq \lambda_k(A),$$

where  $\sup$  denotes the supremum for  $p$ -vectors  $\gamma$  satisfying  $L^* \gamma = 0$ .

A sufficient condition for equality to hold is

$$M(L) \supset M_k(A),$$

which is also a necessary condition when  $k = p$  and which implies that  $M(L)$  is orthogonal to some eigenvector of the matrix  $A$  corresponding to the smallest eigenvalue  $\lambda_p(A)$ .

Proof. The result follows immediately from Lemmas 2 and 3.

Lemma 5. Let  $A, B, A-B$  all belong to  $\mathcal{A}$  and let the rank of  $B$  be less than or equal to  $k$ . Then for each  $i = 1, 2, \dots, p$ ,

$$\lambda_i(A-B) \geq \lambda_{k+i}(A)$$

where  $\lambda_j(A)$  is defined to be zero for  $j > p$ .

Proof. Define  $A_1, A_2, B_1, B_2, C_1$  and  $C_2$  as follows

$$A = A_1 + iA_2, \quad B = B_1 + iB_2, \quad \text{and} \quad C_1 = \begin{pmatrix} A_1 & -A_2 \\ A_2 & A_1 \end{pmatrix}, \quad C_2 = \begin{pmatrix} B_1 & -B_2 \\ B_2 & B_1 \end{pmatrix}.$$

Note that  $A_1$  and  $B_1$  are real symmetric  $p \times p$  matrices,  $A_2$  and  $B_2$  are real skew symmetric  $p \times p$  matrices, and  $C_1$  and  $C_2$  are real symmetric  $2p \times 2p$  matrices. Then  $\{\lambda_i(C_1)\} = \{\lambda_i(A)\}$  and  $\{\lambda_i(C_2)\} = \{\lambda_i(B)\}$  since each eigenvalue of  $A$  (or  $B$ ) occurs exactly twice as an eigenvalue of  $C_1$  (or  $C_2$ ). Thus the rank of  $B$  is less than or equal to  $k$  if and only if the rank of  $C_2$  is less than or equal to  $2k$ , since  $\lambda_{k+1}(B) = 0$  if and only if  $\lambda_{2k+1}(C_2) = \lambda_{2k+2}(C_2) = 0$ . Since  $C_1, C_2$  and  $C_1 - C_2$  are all real symmetric non-negative definite  $p \times p$  matrices, and the rank of  $C_2$  is at most  $2k$ ,

$$\lambda_i(C_1 - C_2) \geq \lambda_{2k+i}(C_1) \quad \text{for } i = 1, 2, \dots, 2p.$$

This result is referred in Okamoto and Kanazawa (1968, p. 860) to Lemma 3. Let  $\Lambda(A)$  represent the diagonal matrix with the eigenvalues of  $A$  in order of decreasing magnitude as the diagonal elements. Then

$\Lambda(C_1), \Lambda(C_2)$  and  $\Lambda(C_1 - C_2)$  are given by

$$\Lambda(C_1) = \begin{pmatrix} \lambda_1(A) & 0 & 0 & \dots & 0 \\ 0 & \lambda_1(A) & 0 & \dots & 0 \\ 0 & 0 & \lambda_2(A) & & \\ \vdots & \vdots & & \ddots & \\ 0 & 0 & & & \lambda_p(A) \end{pmatrix},$$

$$\Lambda(C_1) = \begin{pmatrix} \lambda_1(B) & 0 & 0 & \dots & 0 \\ 0 & \lambda_1(B) & 0 & \dots & 0 \\ 0 & 0 & \lambda_2(B) & & \\ \vdots & \vdots & & \ddots & \\ & & & \lambda_k(B) & 0 \\ & & & & \ddots & \\ 0 & 0 & & & & 0 \end{pmatrix},$$

$$\Lambda(C_1 - C_2) = \begin{pmatrix} \lambda_1(A-B) & 0 & 0 & \dots & 0 \\ 0 & \lambda_1(A-B) & 0 & \dots & 0 \\ 0 & 0 & \lambda_2(A-B) & & \\ \vdots & \vdots & & \ddots & \\ 0 & 0 & & & \lambda_p(A-B) \end{pmatrix}.$$

Thus for  $i = 2, 4, \dots, 2p$ ,  $\lambda_i(C_1) = \lambda_{\frac{i}{2}}(A)$ ,  $\lambda_i(C_2) = \lambda_{\frac{i}{2}}(B)$ , and

$\lambda_i(C_1 - C_2) = \lambda_{\frac{i}{2}}(A-B)$ ; and for  $i = 1, 3, \dots, 2p-1$ ,  $\lambda_i = \lambda_{i+1}$  for  $C_1, C_2$  or

$C_1 - C_2$ . It follows that  $\lambda_{\frac{i}{2}}(A-B) \geq \lambda_{k+\frac{i}{2}}(A)$  for  $i = 2, 4, \dots, p$  and

$\lambda_{\frac{i+1}{2}}(A-B) = \lambda_{\frac{i}{2}}(A-B)$  for  $i = 1, 3, \dots, 2p-1$ .

**Lemma 6.** A necessary and sufficient condition that the equality sign in Lemma 5 holds simultaneously for all  $i$  is that both Hermitian matrices  $A$  and  $B$  can be reduced simultaneously into canonical forms (i.e., there

exists a unitary  $p \times p$  matrix  $T$  and a diagonal matrix  $\Lambda$  with diagonal elements in order of decreasing magnitude such that  $A = T\Lambda T^*$  and  $B = T\Lambda J T^*$  for some matrix  $J$  which can be partitioned into an identity matrix of order not exceeding  $k$  and zero matrices).

Proof. Define  $C_1$  and  $C_2$  as in the proof of Lemma 5. Then it is asserted that  $C_1$  and  $C_2$  can be diagonalized simultaneously if and only if  $A$  and  $B$  can be diagonalized simultaneously.

(i) Let  $T$  be a unitary matrix which simultaneously diagonalizes  $C_1$  and  $C_2$ . That is,  $T$  satisfies  $C_1 = T\Lambda^{(2)}T$  and  $C_2 = T\Lambda^{(2)}J^{(2)}T'$ , where  $\Lambda^{(2)}$  denotes a diagonal matrix with diagonal elements in descending order and with  $\lambda_{11}^{(2)} = \lambda_{22}^{(2)}$ ,  $\lambda_{33}^{(2)} = \lambda_{44}^{(2)}$ , ...,  $\lambda_{(2p-1)(2p-1)}^{(2)} = \lambda_{(2p)(2p)}^{(2)}$ . Then  $T'C_1T = \Lambda^{(2)}$ ; and if  $T$  is partitioned into  $T_1$  and  $T_2$ , each  $p \times 2p$ , it follows that  $\Lambda = T_1'A_1T_1 + T_2'A_2T_1 - T_1'A_2T_2 + T_2'A_1T_2$ , where  $\Lambda$  is the  $p \times p$  diagonal matrix with diagonal elements  $\lambda_{22}, \lambda_{44}, \dots, \lambda_{(2p)(2p)}$ . Letting small letters denote the elements of the matrices, it follows that

$$\begin{aligned} \lambda_{2\ell}^{(2)} = & \sum_h t_{h\ell}^{(1)} \sum_j t_{j\ell}^{(1)} a_{jh}^{(1)} + \sum_h t_{h\ell}^{(1)} \sum_j t_{j\ell}^{(2)} a_{jh}^{(2)} - \sum_h t_{h\ell}^{(2)} \sum_j t_{j\ell}^{(1)} a_{jh}^{(2)} + \\ & + \sum_h t_{h\ell}^{(2)} \sum_j t_{j\ell}^{(2)} a_{jh}^{(1)}. \end{aligned}$$

Using symmetry, this expression reduces to  $\lambda_{2\ell}^{(2)} = \sum_h t_{h\ell}^{(1)} \sum_j t_{j\ell}^{(1)} a_{jh}^{(1)} + \sum_h t_{h\ell}^{(2)} \sum_j t_{j\ell}^{(2)} a_{jh}^{(1)}$ . Since  $A$  is Hermitian, there exists a unitary matrix

$P$  such that  $A = PAP^*$  and hence  $\Lambda = P^*AP$ . Define  $P_1$  and  $P_2$  by  $P = P_1 + iP_2$ . Then  $\lambda_\ell = \sum_h (p^{(1)}_{h\ell} + ip^{(2)}_{h\ell}) \sum_j (p^{(1)}_{jh} - ip^{(2)}_{jh}) (a^{(1)}_{jh} + ia^{(2)}_{jh})$ ,

which can be written

$$\lambda_\ell = \sum_h p^{(1)}_{h\ell} \sum_j p^{(1)}_{jh} a^{(1)}_{jh} + \sum_h p^{(2)}_{h\ell} \sum_j p^{(2)}_{jh} a^{(1)}_{jh} + i \left[ \sum_h p^{(1)}_{h\ell} \sum_j p^{(1)}_{jh} a^{(2)}_{jh} + \sum_h p^{(2)}_{h\ell} \sum_j p^{(2)}_{jh} a^{(2)}_{jh} \right].$$

It has already been established that  $\lambda_{2\ell}^{(2)} = \lambda_\ell$ . Hence  $T = \begin{pmatrix} P_1 & -P_2 \\ P_2 & P_1 \end{pmatrix}$  establishes the relationship between  $T$  and  $P$ , which may, of course, vary by an orthogonal prefactor to  $T$ . If  $R$  is a unitary matrix which diagonalizes  $B$ , it is clear that a similar relationship between  $T$  and  $R$  must hold.

Assume that  $T$  diagonalizes  $C_1$  and  $C_2$  simultaneously. Let  $P$  diagonalize  $A$ . Then there exists an orthogonal matrix  $O$  such that  $OT = \begin{pmatrix} P_1 & -P_2 \\ P_2 & P_1 \end{pmatrix}$ . Then  $OT$  also diagonalizes  $C_1$  and  $C_2$  simultaneously. Hence  $T$  must diagonalize  $B$ .

(ii) Let  $P$  diagonalize  $A$  and  $B$  simultaneously. Then  $T = \begin{pmatrix} P_1 & -P_2 \\ P_2 & P_1 \end{pmatrix}$  diagonalizes  $C_1$  and  $C_2$  simultaneously using the reasoning in (i).

Thus the case for Hermitian matrices has been reduced to a case for real symmetric nonnegative definite matrices for which the result has already been proved.

Theorem. Let  $A$  be any (complex or real)  $p \times k$  matrix and let  $y = (y_1, y_2, \dots, y_k)'$  be any random (complex or real) vector. Let  $f$  be a real-valued function on  $\mathcal{A}$  which is strictly increasing and invariant under any orthogonal transformation in the sense of Lemma 1. Then

$$F_1 = f[E(x - Ay)(x - Ay)^*]$$

is minimized with respect to  $A$  and  $y$  when and only when

$$Ay = \gamma_1 \gamma_1^* x + \gamma_2 \gamma_2^* x + \dots + \gamma_k \gamma_k^* x$$

and the minimum value of  $F_1$  is  $g(\lambda_{k+1}, \dots, \lambda_p, 0, \dots, 0)$ , where  $\gamma_j$  for  $j = 1, 2, \dots, k$  are orthonormal eigenvectors of  $\Sigma$  corresponding to the  $\lambda_j$ 's and  $g$  is the function introduced in Lemma 1.

Note that this theorem does not necessarily hold under the single assumption that  $f$  is strictly increasing, and also that the  $Ay$  which obtains the minimum of  $F_1$  is uniquely determined when and only when  $\lambda_k \neq \lambda_{k+1}$ .

Proof. Let  $r$  be the rank of the matrix  $\Sigma$ . If  $r \leq k$ , the problem is trivial;  $F_1$  is minimized uniquely by taking  $Ay = x$ . Suppose, therefore,  $r > k$ .

Without loss of generality, it is assumed that  $E(yy^*) = I_k$ , and let  $E(xy^*) = B$ . Since  $\begin{pmatrix} \Sigma & B \\ B^* & I_k \end{pmatrix}$  is the covariance matrix of a joint random vector  $\begin{pmatrix} x \\ y \end{pmatrix}$ , both it and  $\Sigma - BB^*$  are Hermitian. Since

$$E[(x - Ay)(x - Ay)^*] = \Sigma - BB^* + (A - B)(A - B)^* \geq \Sigma - BB^*,$$

it follows that  $f[E(x-Ay)(x-Ay)^*] \geq f(\Sigma - BB^*) = F_2$ , say, with the equality sign if and only if  $A = B$ .

By Lemma 1,  $F_2$  is an increasing function of each eigenvalue of  $\Sigma - BB^*$ , which is to be minimized here. Lemmas 5 and 6 imply that  $\lambda_1(\Sigma - BB^*) \geq \lambda_{k+1}(\Sigma)$  for each  $i$ , where the equality holds for all  $i$  simultaneously if and only if  $BB^* = \lambda_1 \gamma_1 \gamma_1^* + \lambda_2 \gamma_2 \gamma_2^* + \dots + \lambda_k \gamma_k \gamma_k^*$ , where the  $\gamma_j$ 's are orthonormal eigenvectors of  $\Sigma$  corresponding to the  $\lambda_j$ 's ( $j = 1, 2, \dots, p$ ). Let  $\Gamma = (\gamma_1, \gamma_2, \dots, \gamma_p)$  and  $\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_p)$ . Then  $BB^*$  can be written as  $BB^* = \Gamma \Lambda^{\frac{1}{2}} \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix} \Lambda^{\frac{1}{2}} \Gamma^*$ . Let  $\tilde{\Lambda}$  denote the diagonal matrix obtained by substituting ones for zeroes in the diagonal of  $\Lambda$ , and define  $Q$  by  $Q = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} = \tilde{\Lambda}^{-\frac{1}{2}} \Gamma^* B$ , where  $Q$  is a  $k \times k$  matrix and  $Q_2$  is a  $(p-k) \times p$  matrix. Then  $\begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix} = QQ^* = \begin{pmatrix} Q_1 Q_1^* & Q_1 Q_2^* \\ Q_2 Q_1^* & Q_2 Q_2^* \end{pmatrix}$ , and hence  $Q_1 Q_1^* = I_k$  and  $Q_2 = 0$ . Therefore  $F_2$  is minimized by taking  $B = \Gamma \tilde{\Lambda}^{\frac{1}{2}} \begin{pmatrix} Q_1 \\ 0 \end{pmatrix} = G$ , say, where  $Q_1$  is any unitary  $k \times k$  matrix and the minimum value of  $F_2$  is

$$\begin{aligned} & f(\lambda_{k+1} \gamma_{k+1} \gamma_{k+1}^* + \lambda_{k+2} \gamma_{k+2} \gamma_{k+2}^* + \dots + \lambda_p \gamma_p \gamma_p^*) \\ & = g(\lambda_{k+1}, \lambda_{k+2}, \dots, \lambda_p, 0, \dots, 0), \end{aligned}$$

where  $g$  is the function defined in Lemma 1. Define  $H$  by  $H = \Gamma \tilde{\Lambda}^{-\frac{1}{2}} \begin{pmatrix} Q_1 \\ 0 \end{pmatrix}$  and  $\gamma = H^* x$ . Then it is easily seen that  $\Sigma H = G$  and  $H^* G = I_k$ . Now

it is asserted that there exists uniquely a random vector  $y$  satisfying the conditions  $E(yy^*) = I_k$  and  $E(xy^*) = G$ . In fact,  $y$  is the solution, for  $E(xy^*) = E(xx^*)H = \Sigma H = G$  and  $E(yy^*) = H^* E(xy^*) = H^* G = I_k$ .

Uniqueness follows from the fact  $E(y-y)(y-y)^* = E(yy^*) - E(yy^*) -$

$$E(y^*y) + E(yy^*) = I_k - I_k = I_k + I_k = 0,$$

since  $E(yy^*) = H^* E(xy^*) = H^* G$ . Thus  $F_1$  is minimized by taking

$$Ay = Gy = GH^*x = \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix} \Gamma^* x = \gamma_1 \gamma_1^* x + \gamma_2 \gamma_2^* x + \dots + \gamma_p \gamma_p^* x.$$



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## APPENDIX

$$\Phi_{k\ell}(t, u) \Big|_{\substack{t=\frac{1}{2}(\mu_1-\mu_2) \\ u=1}} \quad \text{for } k, \ell = 0, 1, 2, 3, 4.$$

Let  $\Phi_{k\ell}(t, u) \Big|_{\substack{t=\frac{1}{2}(\mu_1-\mu_2) \\ u=1}}$  be denoted in this appendix by  $\Phi_{k\ell}$ .

Note that  $\Phi_k$  in the text is given in this appendix as  $\Phi_{k0}$ .

$$\Phi_{00} = \Phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{10} = \phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{01} = -\frac{1}{4}(\mu_1 - \mu_2)\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{20} = -\frac{1}{2}(\mu_1 - \mu_2)\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{11} = \left[-\frac{1}{2} + \frac{1}{8}(\mu_1 - \mu_2)^2\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{02} = \left[\frac{3}{8}(\mu_1 - \mu_2) - \frac{1}{32}(\mu_1 - \mu_2)^3\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{30} = \left[-1 + \frac{1}{4}(\mu_1 - \mu_2)^2\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{21} = \left[\frac{3}{4}(\mu_1 - \mu_2) - \frac{1}{16}(\mu_1 - \mu_2)^3\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{12} = \left[\frac{3}{4} - \frac{3}{8}(\mu_1 - \mu_2)^2 + \frac{1}{64}(\mu_1 - \mu_2)^4\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{03} = \left[-\frac{15}{16}(\mu_1 - \mu_2) + \frac{5}{32}(\mu_1 - \mu_2)^3 - \frac{1}{256}(\mu_1 - \mu_2)^5\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{40} = \left[\frac{3}{2}(\mu_1 - \mu_2) - \frac{1}{8}(\mu_1 - \mu_2)^3\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{31} = \left[\frac{3}{2} - \frac{3}{4}(\mu_1 - \mu_2)^2 + \frac{1}{32}(\mu_1 - \mu_2)^4\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{22} = \left[ -\frac{15}{8}(\mu_1 - \mu_2) + \frac{5}{16}(\mu_1 - \mu_2)^3 - \frac{1}{128}(\mu_1 - \mu_2)^5 \right] \phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{13} = \left[ -\frac{15}{8} + \frac{45}{32}(\mu_1 - \mu_2)^2 - \frac{15}{128}(\mu_1 - \mu_2)^4 + \frac{1}{512}(\mu_1 - \mu_2)^6 \right] \phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_{04} = \left[ \frac{105}{32}(\mu_1 - \mu_2) - \frac{105}{128}(\mu_1 - \mu_2)^3 + \frac{21}{512}(\mu_1 - \mu_2)^5 - \frac{1}{2048}(\mu_1 - \mu_2)^7 \right] \cdot \phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_k^{(2)}(t) \Big|_{t=\frac{1}{2}(\mu_1 - \mu_2)} \quad \text{for } k = 0, 1, 2, 3, 4.$$

$$\text{Let } \Phi_k^{(2)}(t) \Big|_{t=\frac{1}{2}(\mu_1 - \mu_2)} \quad \text{be denoted in this appendix by } \Phi_k^{(2)}$$

$$\Phi_0^{(2)} = [\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]]^2$$

$$\Phi_1^{(2)} = 2\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]$$

$$\Phi_2^{(2)} = -(\mu_1 - \mu_2)\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right] + 2(\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right])^2$$

$$\Phi_3^{(2)} = \left[-2 + \frac{1}{2}(\mu_1 - \mu_2)^2\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right] - 3(\mu_1 - \mu_2)(\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right])^2$$

$$\Phi_4^{(2)} = \left[3(\mu_1 - \mu_2) - \frac{1}{4}(\mu_1 - \mu_2)^2\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right]\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right] + \left[-8 + \frac{7}{2}(\mu_1 - \mu_2)^2\right](\phi\left[\frac{1}{2}(\mu_1 - \mu_2)\right])^2.$$

$$\Phi_k(t) \Big|_{k=\frac{1}{2}(\mu_1 - \mu_2)} \quad \text{for } k = 0, 1, 2, 3.$$

Let  $\phi_k(t) \Big|_{t=\frac{1}{2}(\mu_1-\mu_2)}$  be denoted in this appendix by  $\phi_k$ .

$$\phi_0 = \Phi_{10} = \phi\left[\frac{1}{2}(\mu_1-\mu_2)\right]$$

$$\phi_1 = \Phi_{20} = -\frac{1}{2}(\mu_1-\mu_2)\phi\left[\frac{1}{2}(\mu_1-\mu_2)\right]$$

$$\phi_2 = \Phi_{30} = \left[-1 + \frac{1}{4}(\mu_1-\mu_2)^2\right]\phi\left[\frac{1}{2}(\mu_1-\mu_2)\right]$$

$$\phi_3 = \Phi_{40} = \left[\frac{3}{2}(\mu_1-\mu_2) - \frac{1}{8}(\mu_1-\mu_2)^3\right]\phi\left[\frac{1}{2}(\mu_1-\mu_2)\right]$$

$$\phi_k^{(2)}(t) \Big|_{t=\frac{1}{2}(\mu_1-\mu_2)} \quad \text{for } k = 0, 1, 2, 3.$$

Let  $\phi_k^{(2)}(t) \Big|_{t=\frac{1}{2}(\mu_1-\mu_2)}$  be denoted in this appendix by  $\phi_k^{(2)}$ .

$$\phi_0^{(2)} = (\phi\left[\frac{1}{2}(\mu_1-\mu_2)\right])^2$$

$$\phi_1^{(2)} = -(\mu_1-\mu_2)(\phi\left[\frac{1}{2}(\mu_1-\mu_2)\right])^2$$

$$\phi_2^{(2)} = [-2 + (\mu_1-\mu_2)^2](\phi\left[\frac{1}{2}(\mu_1-\mu_2)\right])^2$$

$$\phi_3^{(2)} = [6(\mu_1-\mu_2) - (\mu_1-\mu_2)^3](\phi\left[\frac{1}{2}(\mu_1-\mu_2)\right])^2$$